Data Processing for ICR Abastract

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Chain Number Density, ν

Reported data in Suzuki et al. (2012)

$$\nu \approx 3.7 \times 10^{21}/m^3 \quad \text{number density for active chains} \tag{1}$$

$$\nu_0 = 1.8 \times 10^{23}/m^3 \quad \text{number density for all chains} \tag{2}$$

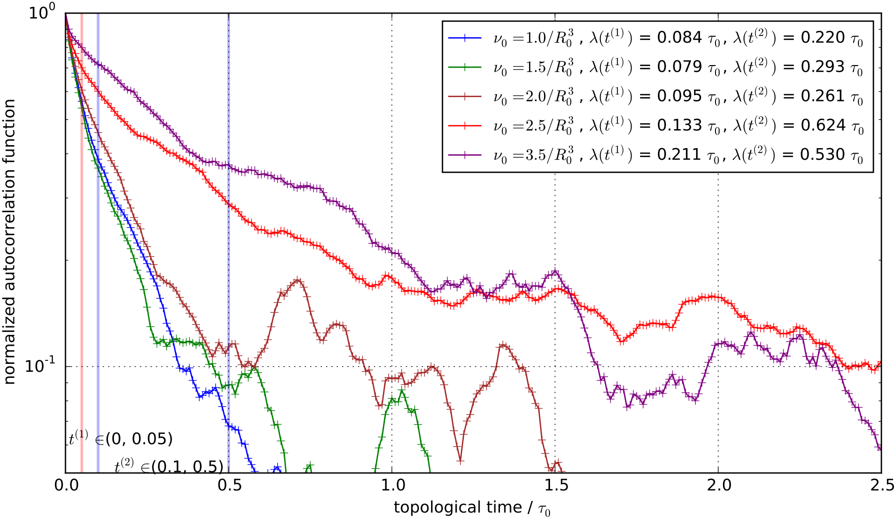
Note that $R_0 \in [10^2, 10^3] nm^3$, which implies $\nu_0 \in 1.8 \times [10^{-1}, 10^2]/R_0^3$.

The given condition:

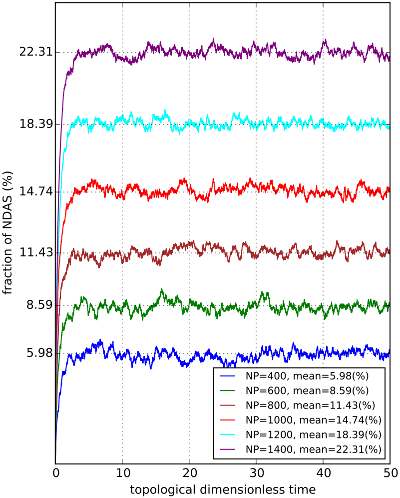
- Number of chains per particles $=$ 25
- Number of particles $=$ 400, 600, 800, 1000, 1200, 1400
- Volume of box $= 10^3 R_0^3$

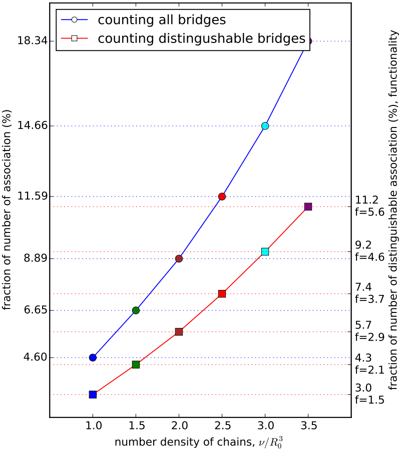
Measured number density: $\nu_0 R_0^3 = \{1,\ 1.5,\ 2,\ 2.5,\ 3,\ 3.5\}$

ACF, legend change



Number of Distingushable Association, Functionality





Relaxation Time Spectrum

Continuous relaxation time spectrum

$$G(t) = \sum_i G_i \exp\left(-\frac{t}{\lambda_i}\right) \quad \Rightarrow \quad G(t) = \int_0^\infty H(\lambda) \exp\left(-\frac{t}{\lambda}\right) d\log\lambda, \tag{3}$$

where $H(\lambda)$ is called relaxation time spectrum.

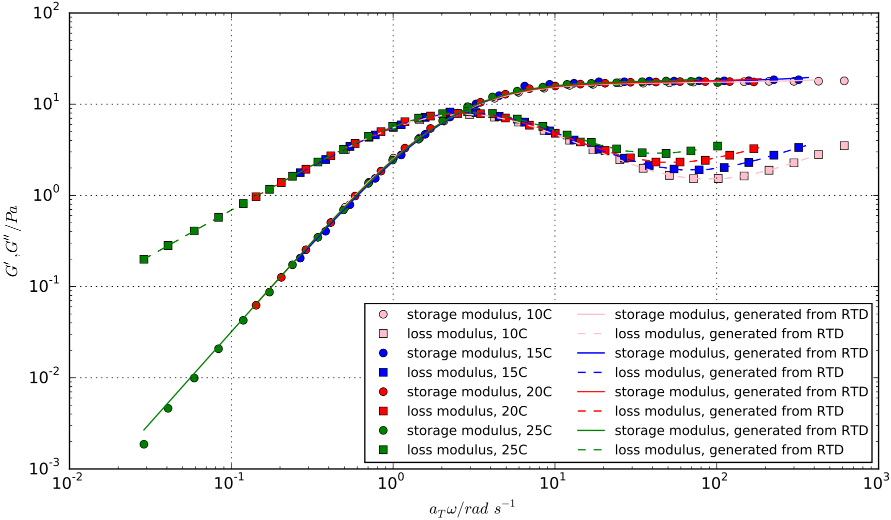
$$G'(\omega) = \int_0^\infty H(\lambda) K'(\lambda\omega) d\log\lambda \tag{4}$$

$$G''(\omega) = \int_0^\infty H(\lambda) K''(\lambda\omega) d\log\lambda \tag{5}$$

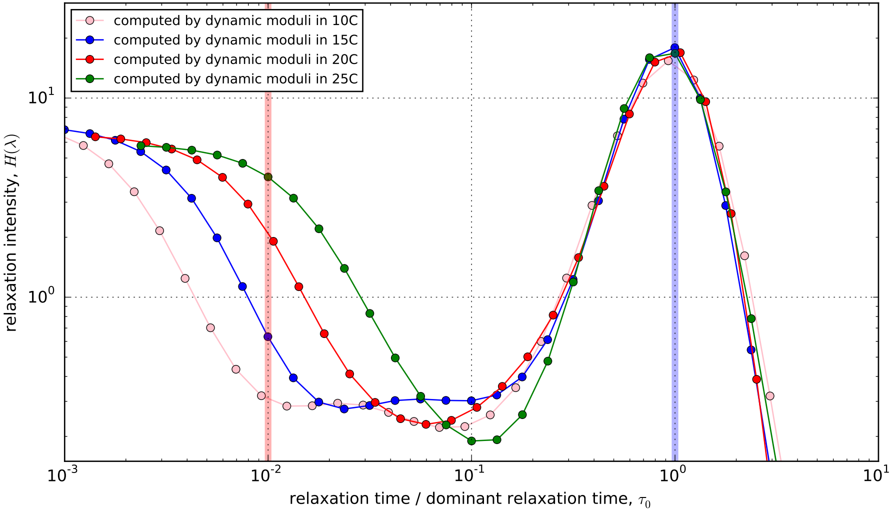
with

$$K'(\lambda\omega) = \frac{\lambda^2\omega^2}{1+\lambda^2\omega^2} \quad K''(\lambda\omega) = \frac{\lambda\omega}{1+\lambda^2\omega^2}. \tag{6}$$

Dynamic Moduli, Reproduced from Suzuki et al. (2012)



Relaxation Time Spectrum, Cho and Park (2013)



Performance Check

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Test Condition, larger time step

Current definition for time scales

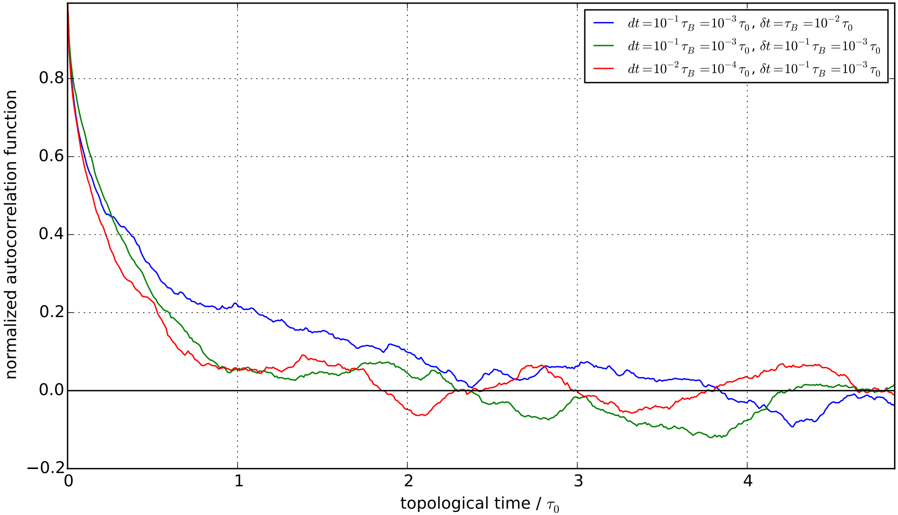
$$\tau_0 = \beta_0^{-1} \quad \text{dissociation time} \tag{7}$$

$$\tau_B = \frac{R_0^2 \zeta}{k_B T} \frac{1}{C}, \quad \text{Brownian time.} \tag{8}$$

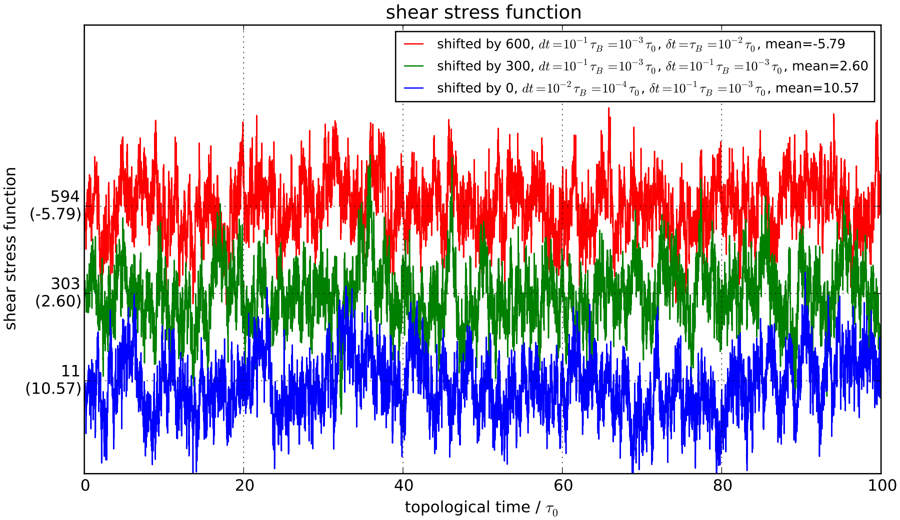
As a default, the rational time scale, $R_t = \tau_0 / \tau_B$, is set by 100.

- time step for Brownian motion: $10^{-4}\tau_0$ $(=10^{-2}\tau_B) \Rightarrow 10^{-3}\tau_0$ $(=10^{-1}\tau_B)$
- time step for topology: $10^{-3}\tau_0 \Rightarrow 10^{-3}\tau_0$ and $10^{-2}\tau_0$
- data output frequency: $10^{-2}\tau_0$

ACF, failed to match



Shear Stress



ACF, failed to match