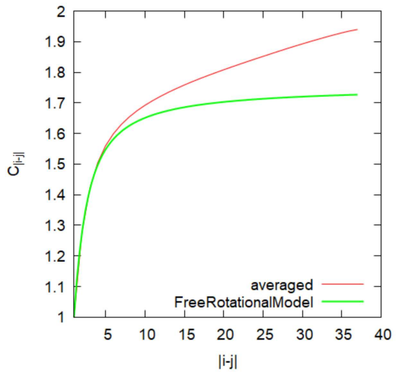
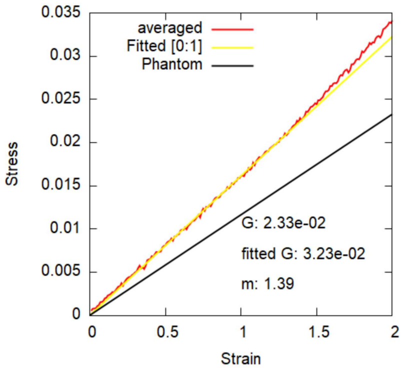
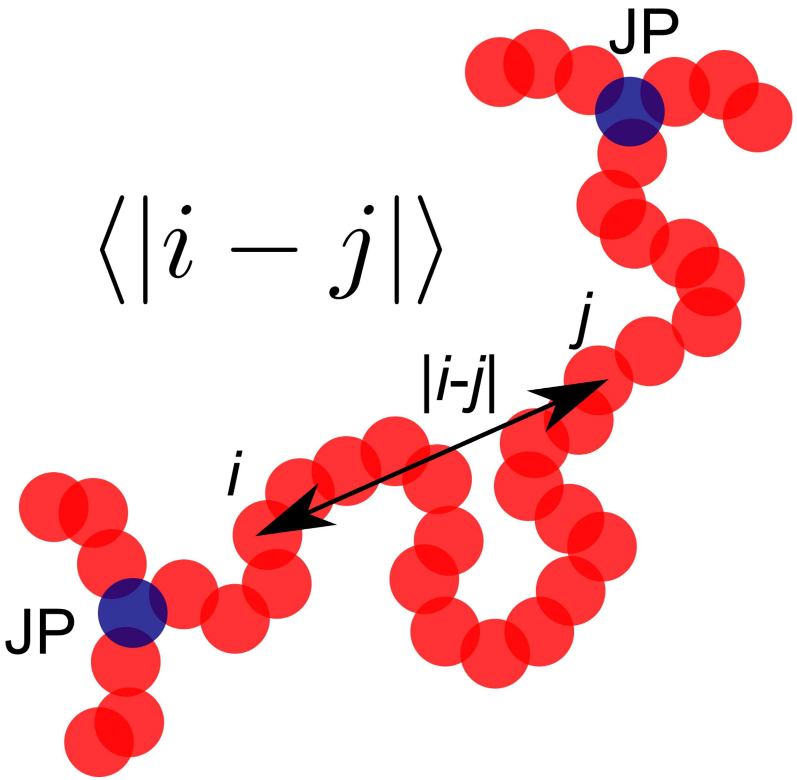
Phantom Chain NW (f=4, N=36)

- Strand-length is set to Equilibrated length (N=36)
- Multiplicity is 3 to keep $\rho = 0.85$

N = 36
Shrinkage = 1.0

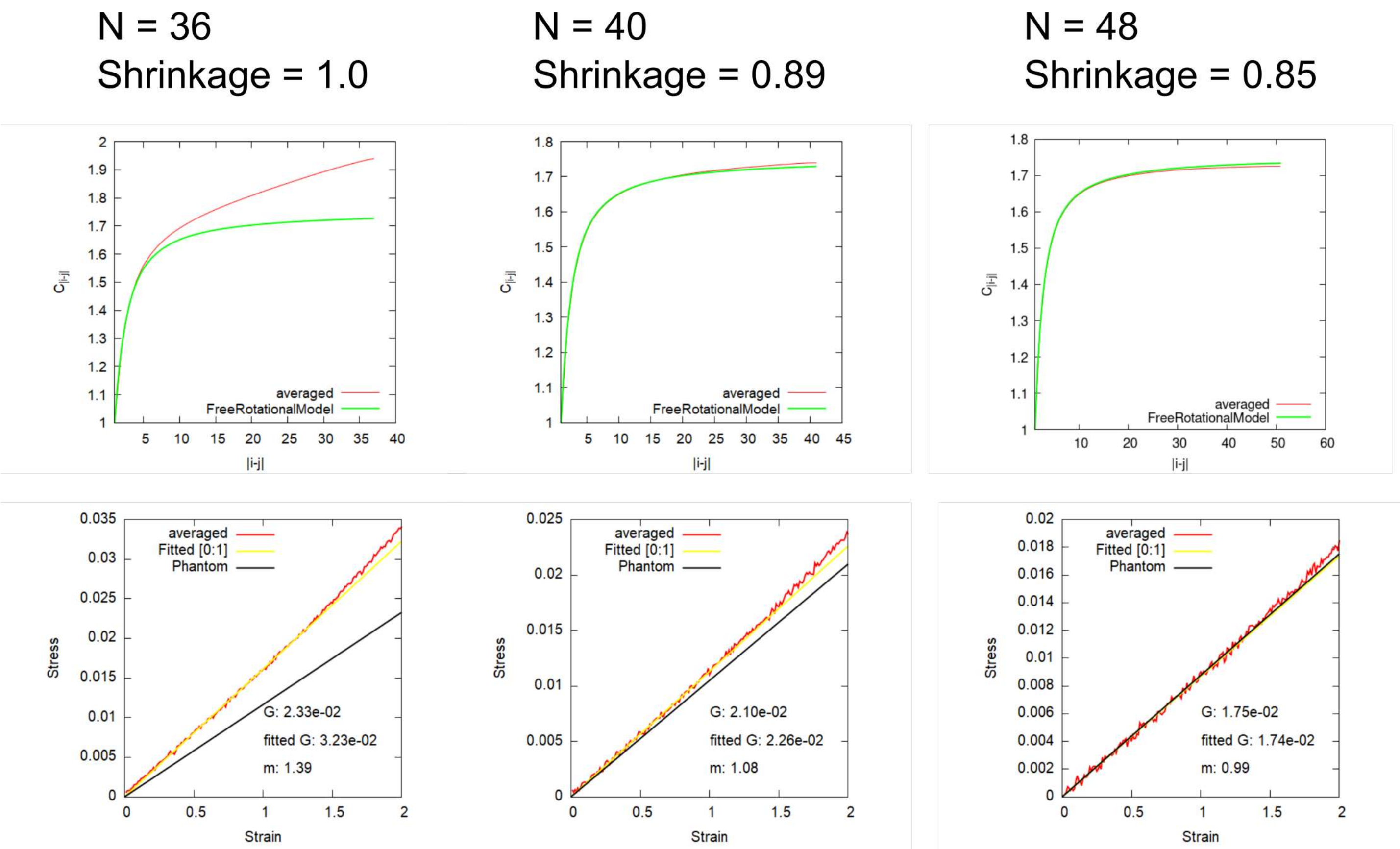






Strand length Effect for Phantom Chain NW

- Strand-length is varied from 36 to 48 for f=4
- System size is reduced to keep $\rho = 0.85$



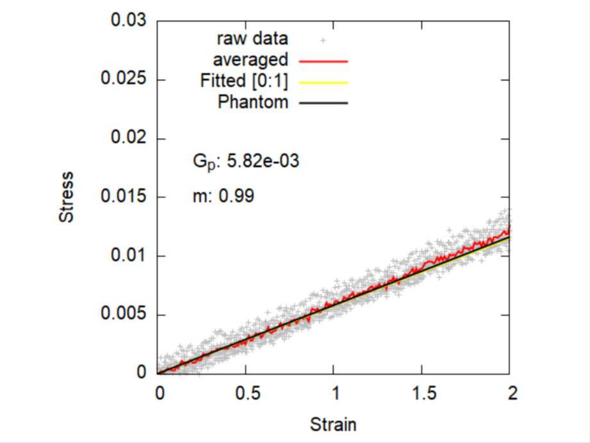
Strand Length Comparison for Shear Stress

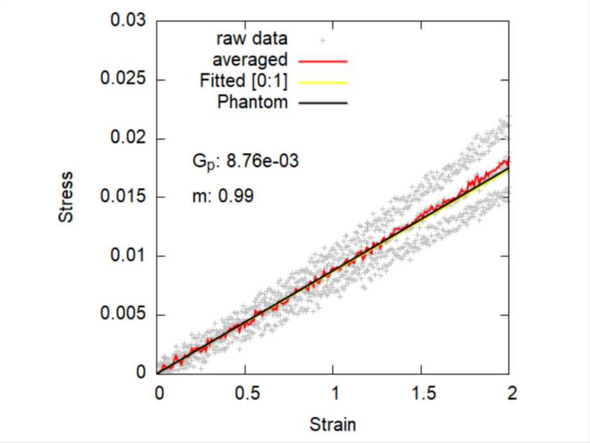
Comparison of Functionality (f = 3, 4, 6)

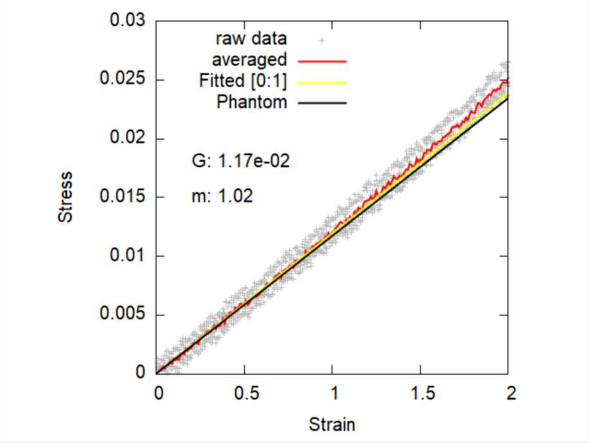
For Varied Functionalities

- With proper strand length
- Modulus changed according to theory

f = 3	f = 4	f = 6
N = 48	N = 48	N = 48
multi = 4	multi = 3	multi = 2





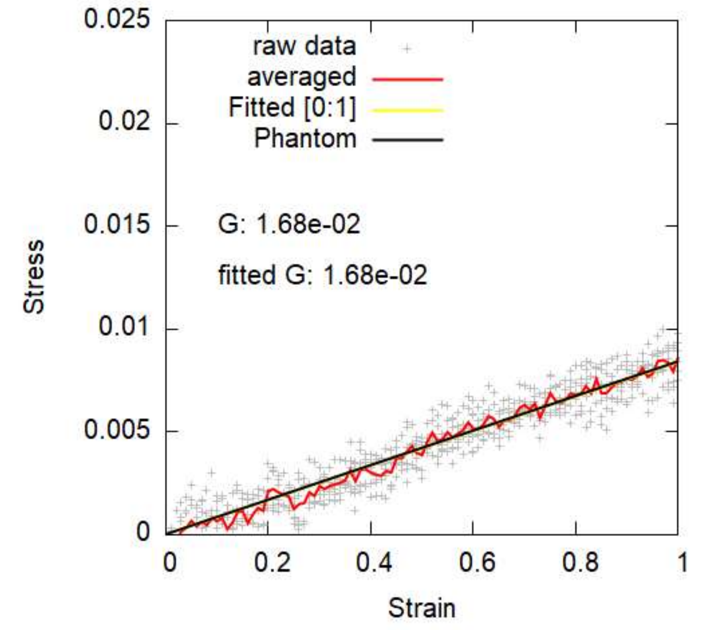


Mechanical Responce for KG Chains(f=4, N=48)

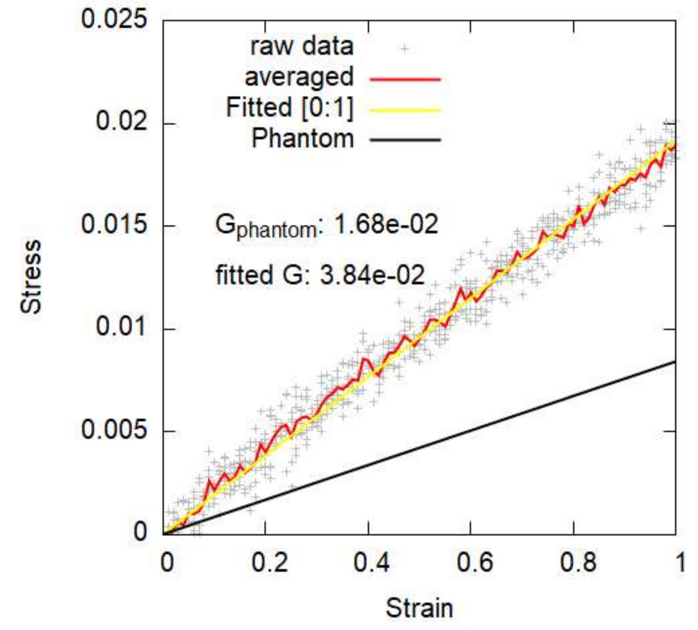
4-Chain Random Network with KG Chain

- Excluded Volume Effect by non-bonding LJ Potential.
- No strands mutual crossing by FENE bond.

Phantom Chain

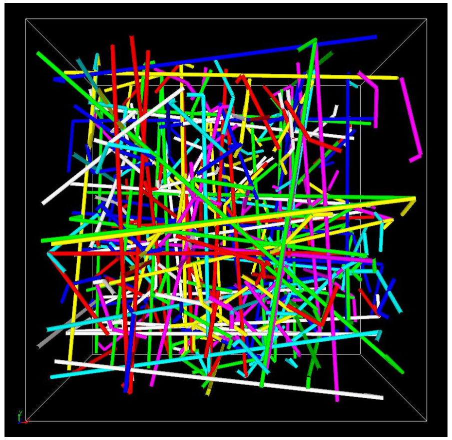


KG Chain

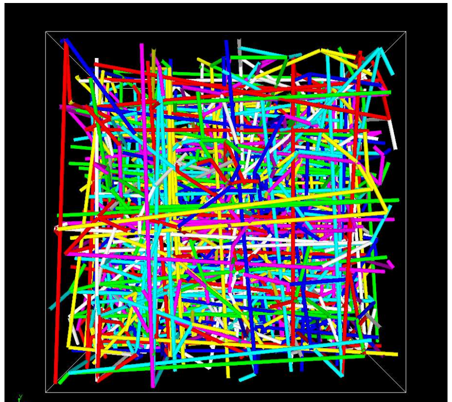


Reduced Entanglements by NPT Model

- 4-Chain-NPT
  $< Z >_{Z1} = 0.36$

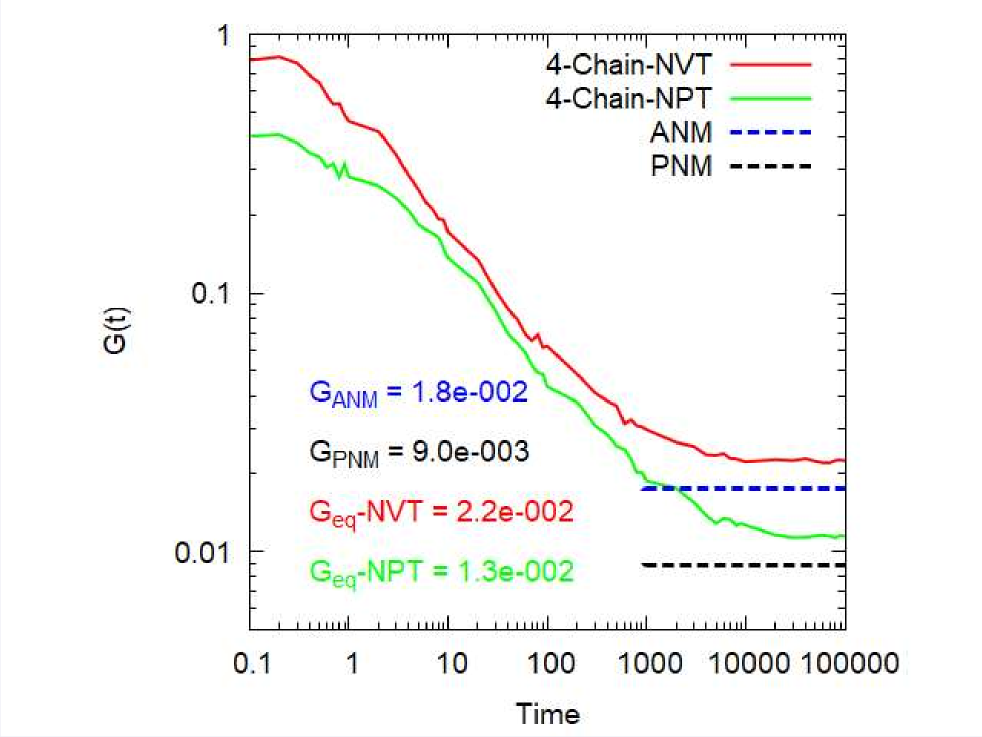


- 4-Chain-NVT
  $< Z >_{Z1} = 1{,}04$



$G(t)$

- Step Deformation $(\lambda = 2.0)$
- Reduced Modulus



Entanglement effect in Slip-tube Model

Entanglement in Slip-tube Model

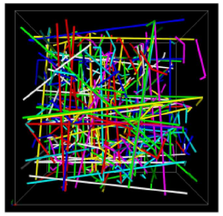
Theoretical model by Rubinstein[a]

$$G_c = \nu k_B T \left(1 - \frac{2}{\phi}\right), \quad G_e = \frac{4}{7}\nu k_B T L$$

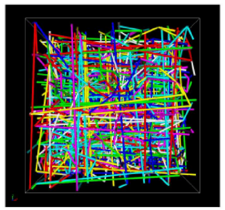
and L is the number of slip-links per network chain

[a] M. Rubinstein, S. Panyukov, Macromolecules, 35, 6670 (2002)

NPT
(less Entgld.)



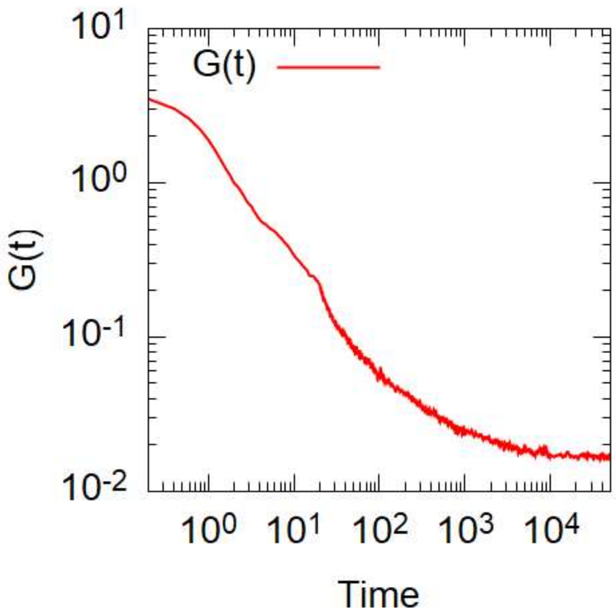
NVT
(well Entgld.)



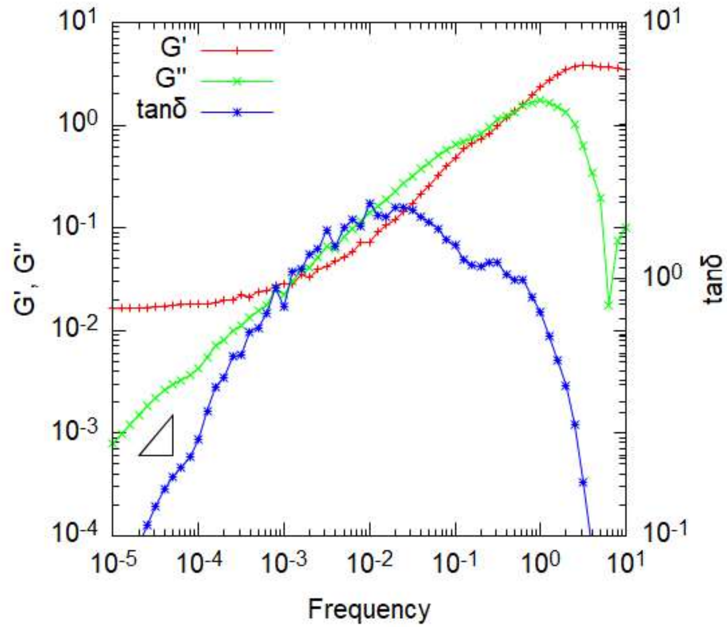
Ensemble	NPT	NVT
Chains, ν	768, 0.018	
$G_c = \nu \times (1 - 2/4)$	0.009	
Entanglements	278	800
Entangled Chains	249	557
L	278/768=0.36	800/768=1.04
$G_e = 4/7 \times \nu \times L$	0.004	0.011
$G_{calcd.} = G_c + G_e$	0.013	0.020
$G_{measd.}$	0.013	0.022

G(t) for Step Shear and Dynamic Rheo-Spectrum

G(t) for Step Stretch



Dynamic Viscoelastics

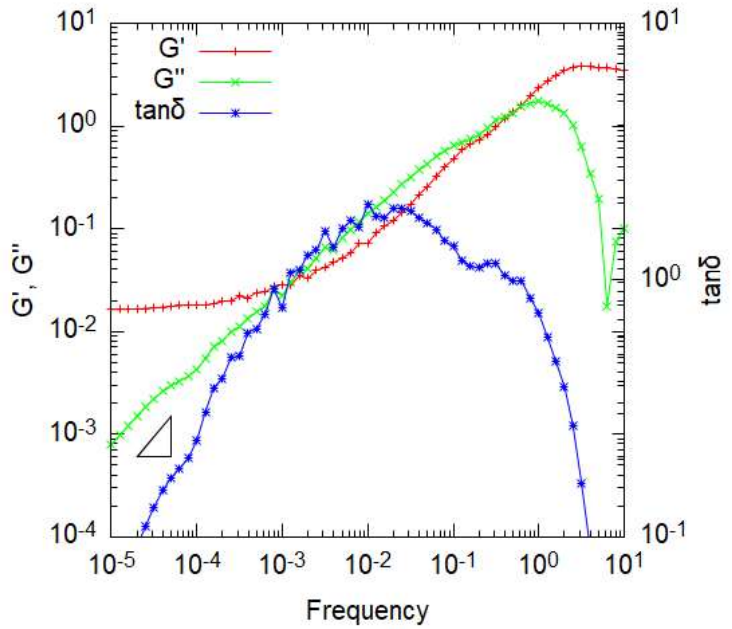


Conditions

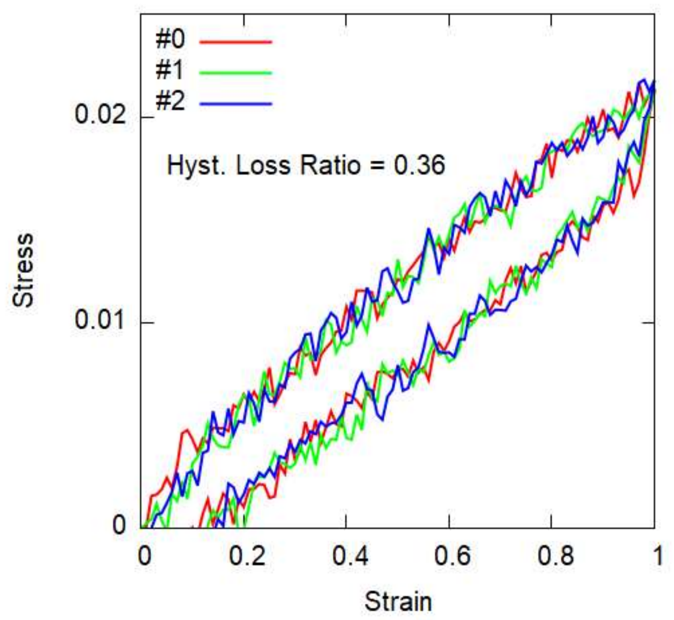
- 4-Chain KG-NW(N=50)
- Step Stretch: $\lambda = 2$
- G(t) is transformed to Dynamic Viscoelastic Spectrum

Mechanical Hysteresis Loss

Dynamic Viscoelastics



Hysteresis by Cyclic Shear



Conditions

- 4-Chain KG-NW(N=50)
- Cyclic Shear: $\gamma = 1$, $\dot{\gamma} = 5e^{-5}$

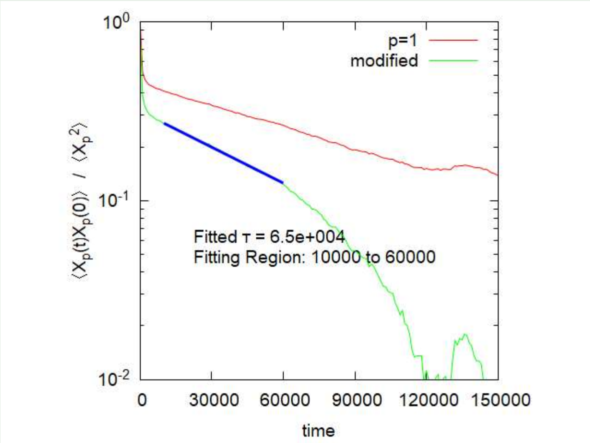
ストランドの最長緩和時間

最長緩和時間 (τ) を評価

- ストランドのラウスモード（p=1）の自己相関関数 $C_p(t)$

$$C_p(t) = \langle X_p(t) X_p(0) \rangle / \langle X_p^2 \rangle$$

- 相関関数の振る舞い
  - 長時間極限で一定値に収束
  - 空間的な拘束のため
  - $C_p(\infty)$ を差し引いて評価



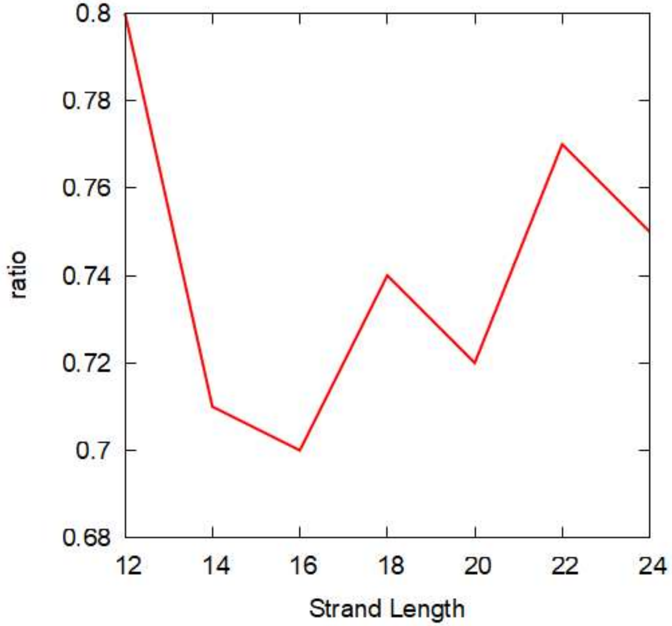
$C_{p1}(t)$ for equilibrated structure

$$\tau \simeq 6.5e^4$$

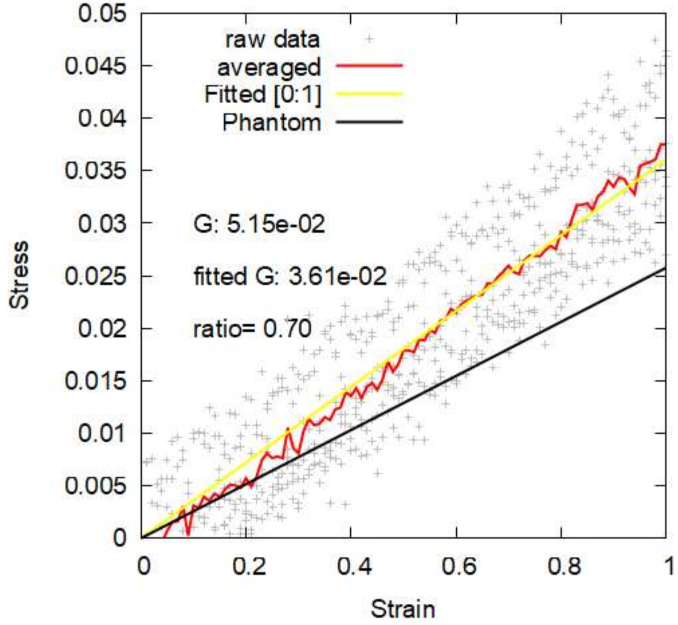
ヒステリシスロスが消失する変形速度 ($\sim 1e^{-5}$) と対応

Effect of Strand Length for Shorter KG Chain

- For Phantom Chain
  - Longer Strand resulted in lower Modulus
- KG Chain
  - Proper Length was found for Low Modulus
  - which implies proper restriction for JP



Strand Length vs. Modulei ratio



Shear Stress for N=16

Conclutions

- Introducing random connectivity, MD simulation studies were carried out.
- To investigate the criteria for Phantom Network Model, Two model chains are used.
  - Employing phantom chain, basics for PNM is examined.
    - Proper strand length is the key for PNM.
    - Functionality effect was confirmed.
  - Changing the chain to KG Chain, constraints effects are investigated.
    - Trapped Entanglement was explained by Slip-tube Model
    - Hysteresis