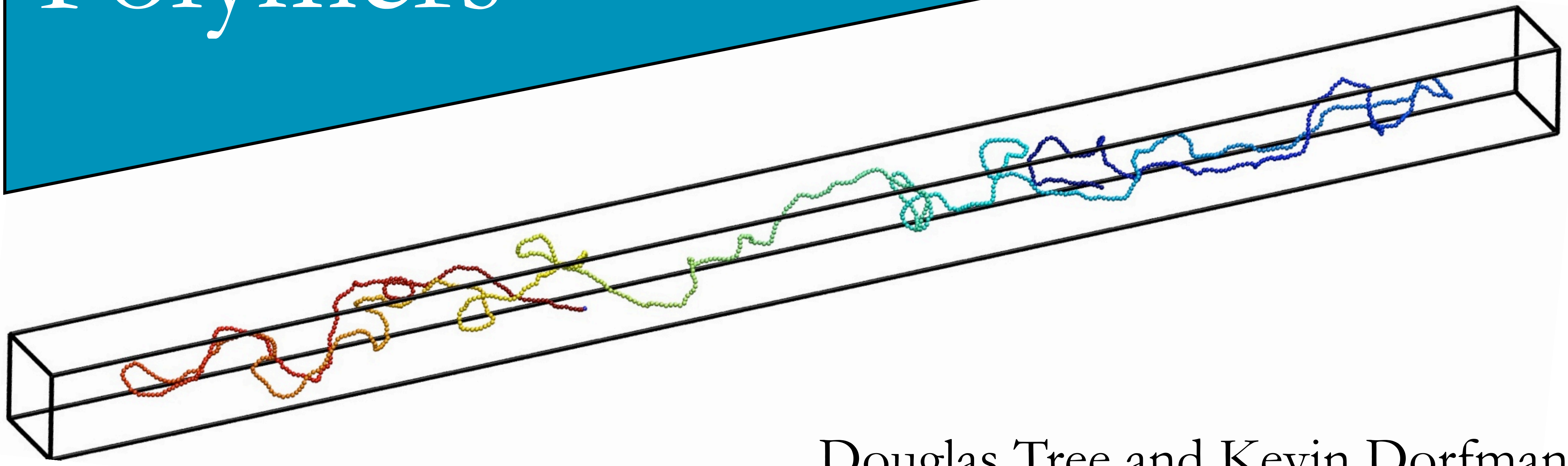
Crossover Behavior in Confined Semiflexible Polymers



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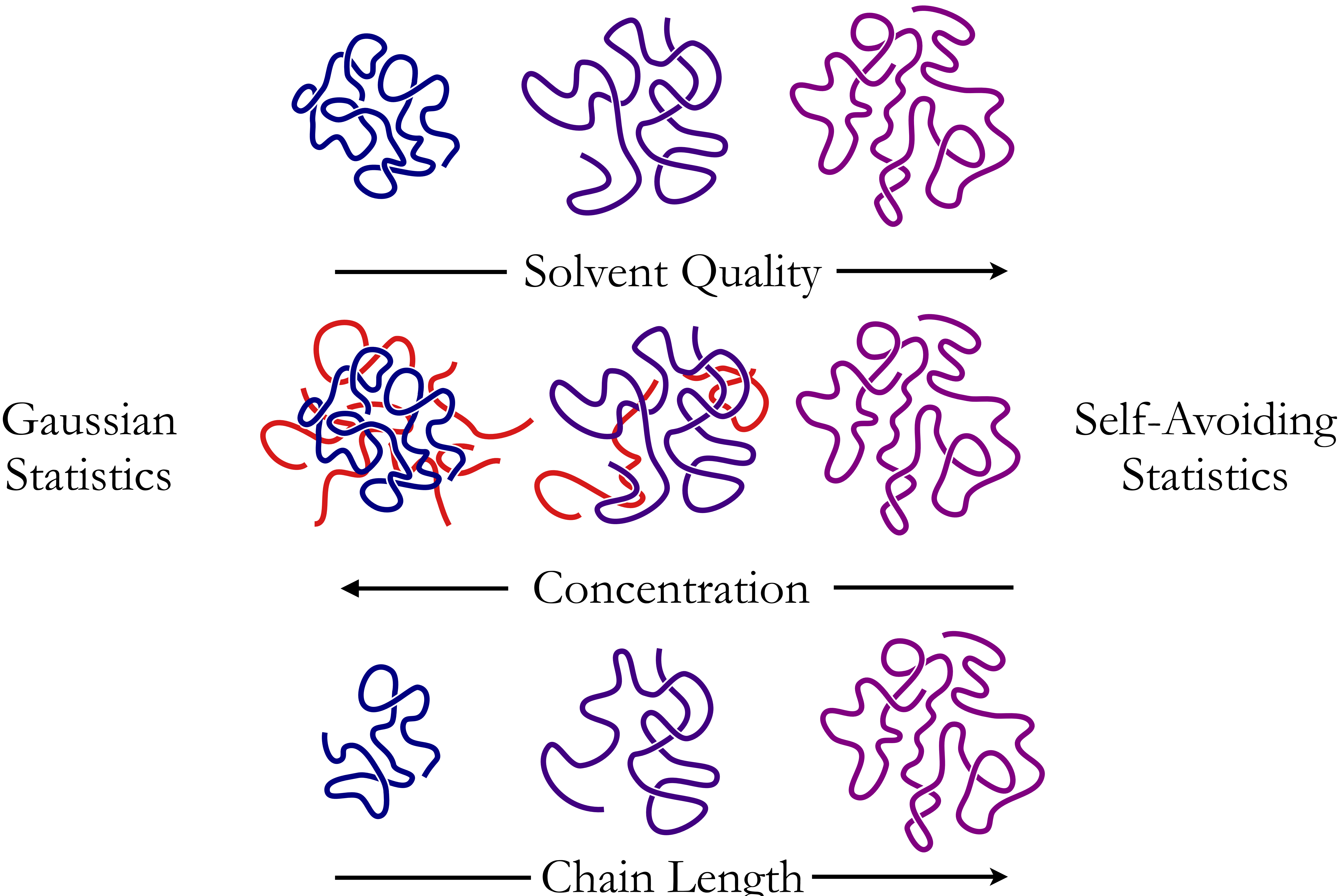
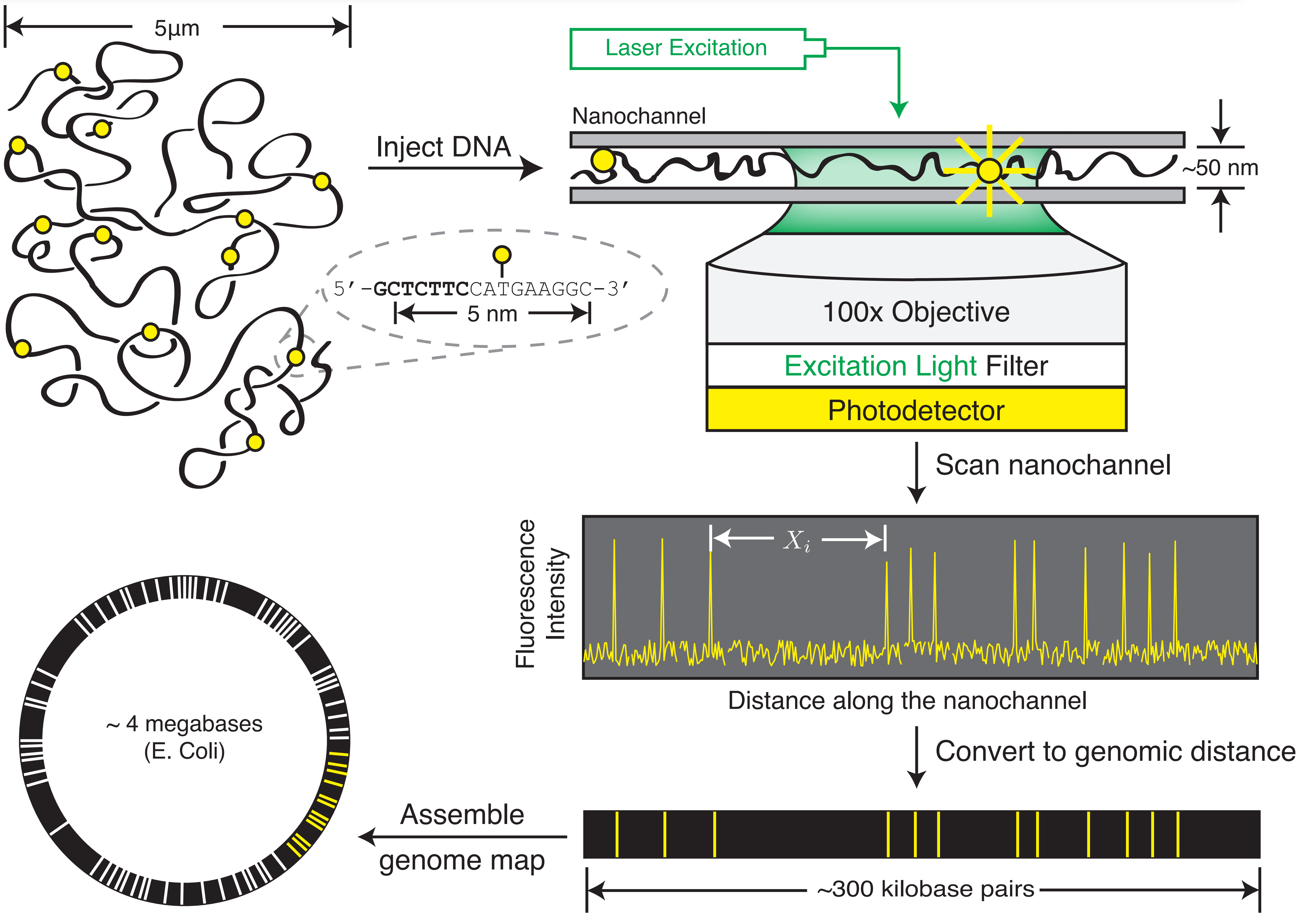
Chem. Eng. and Mat. Sci.

APS March Meeting 2014
Denver, CO

The Excluded Volume Problem

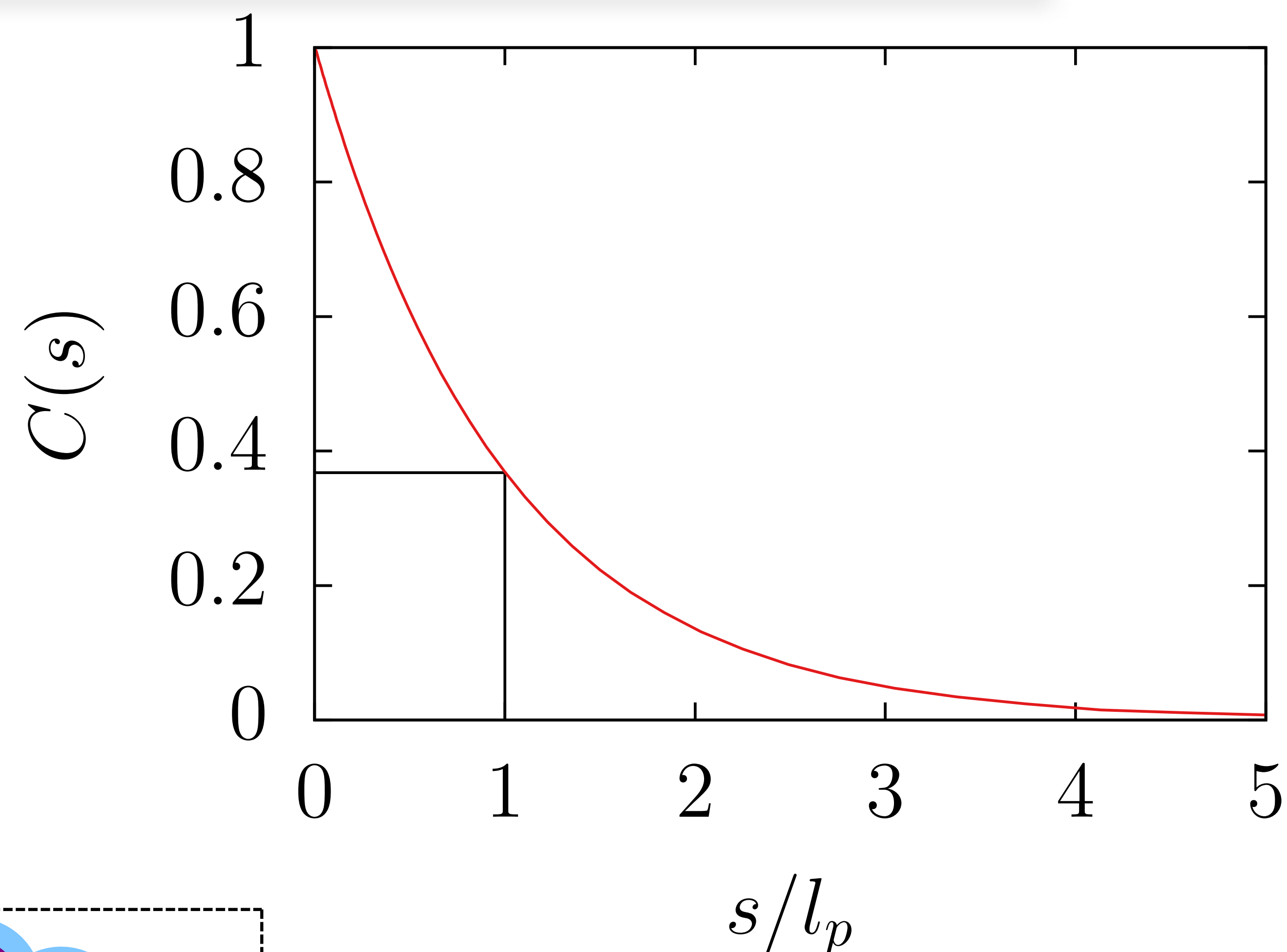


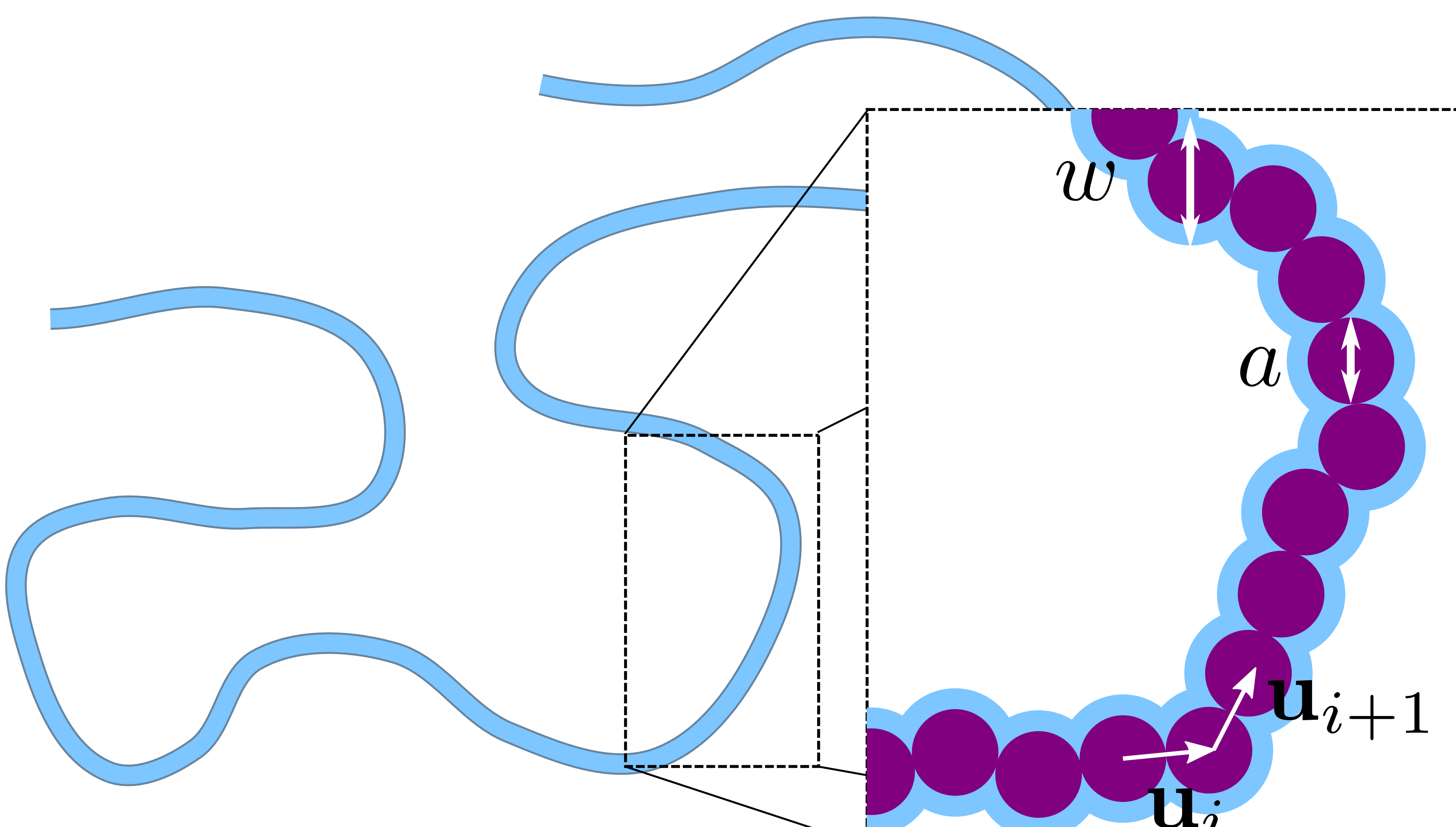
Genomic Mapping



Wormlike Chains (WLC)

- Good description of stiff biopolymers such as dsDNA
- Stiffness characterized by decay of bond correlations, l_p
- Excluded volume characterized by effective width, w





$$C(s) = \langle \mathbf{u}(s) \cdot \mathbf{u}(0) \rangle$$
$$= \exp(-s/l_p)$$

$$l_p = b/2$$

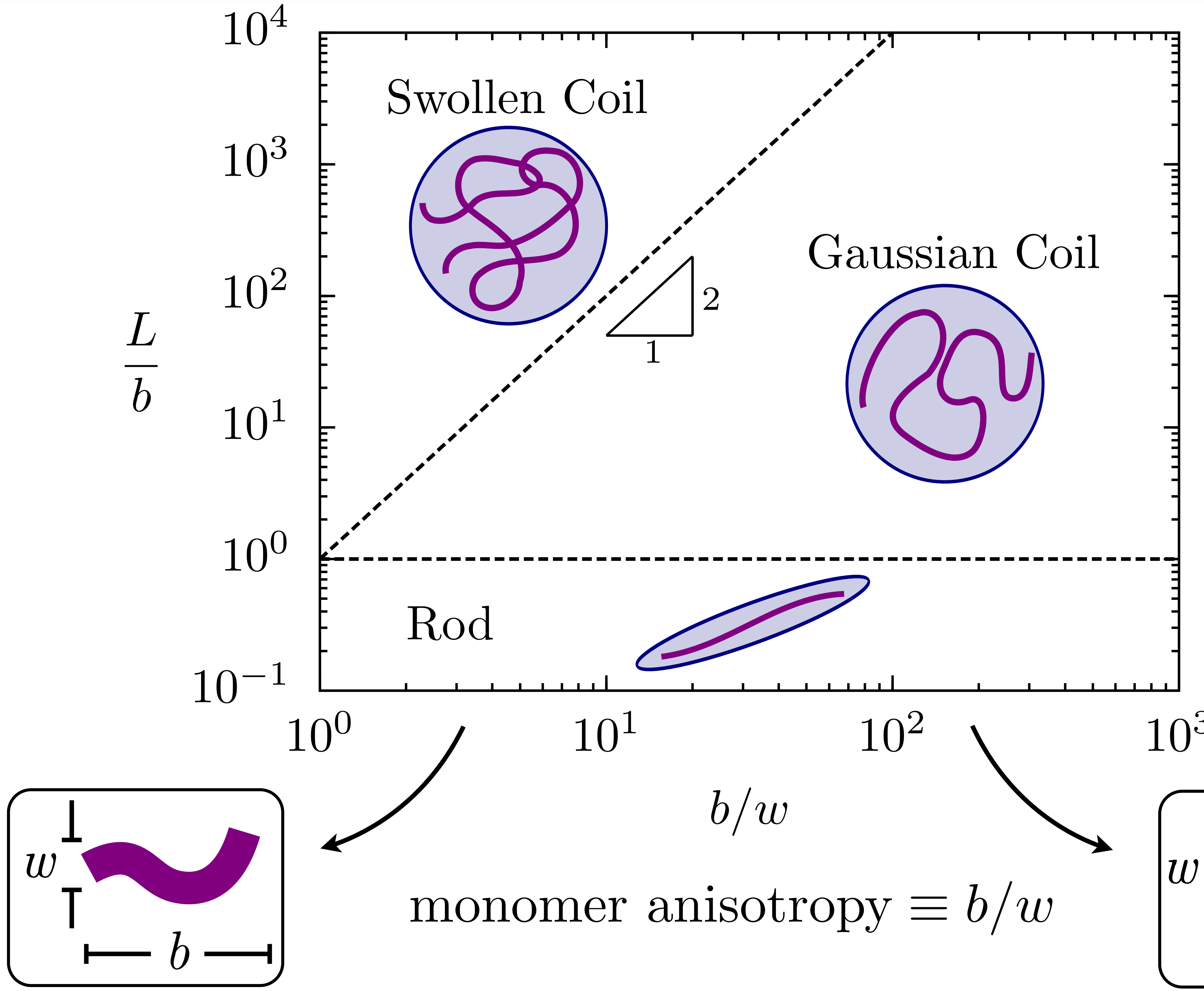
A Numerical Approach

- Traditional Metropolis Monte Carlo is impractical for chains longer than O(10^3) beads.

- Pruned-enriched Rosenbluth Method (PERM)
  - Chain-growth Monte Carlo technique
  - Efficient for O(10^4-10^5) beads
  - Applicable to confined and unconfined systems
  - Off-lattice
  - Can estimate free energies

Tree et al. Macromolecules. (2013)
Grassberger. Phys. Rev. E. (1997).
Prellberg and Krawczyk. Phys. Rev. Lett. (2004).

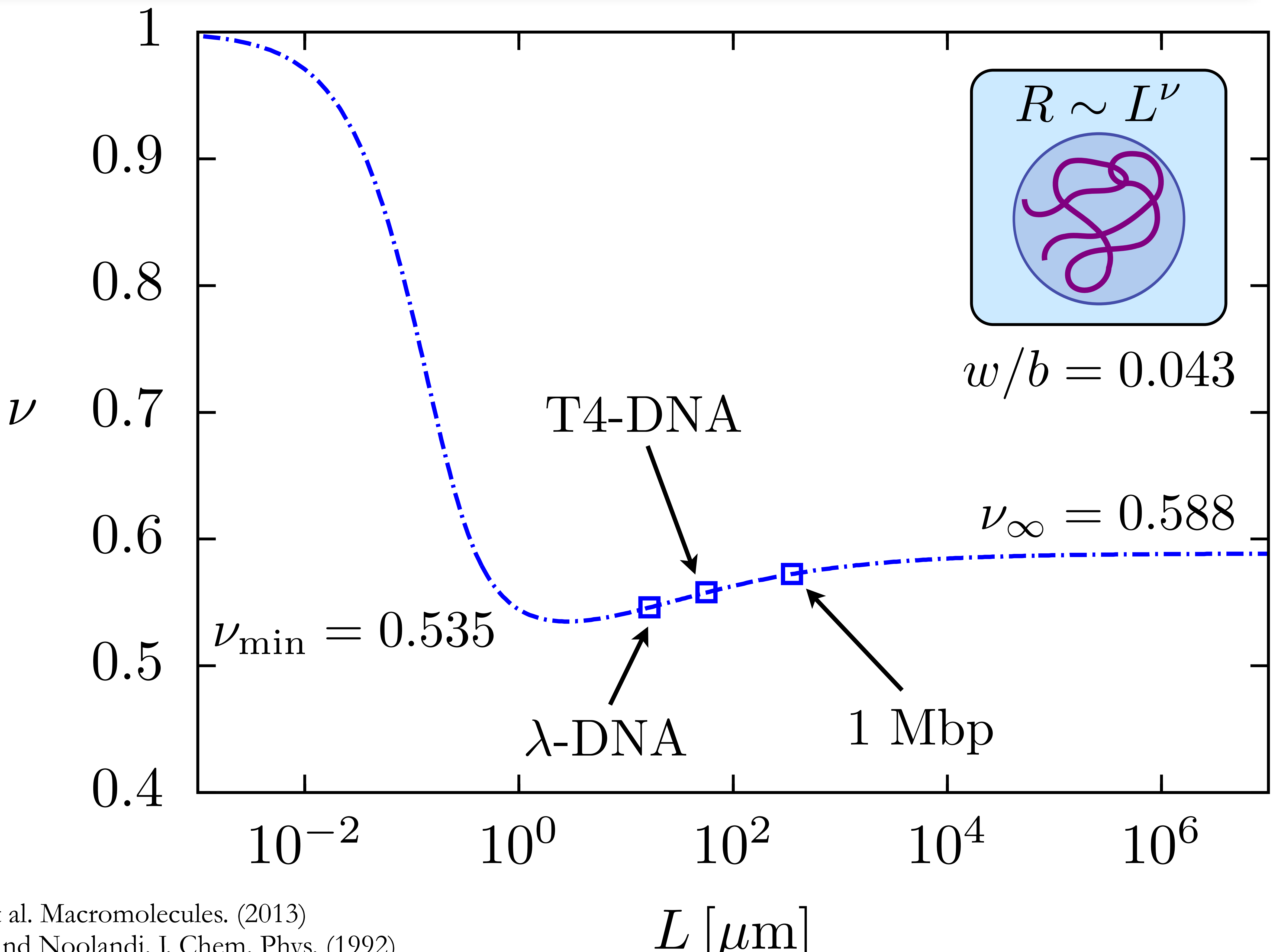
Monomer Anisotropy



Tree et al. Macromolecules. (2013)

$$\text{monomer anisotropy} \equiv b/w$$

Free Solution DNA

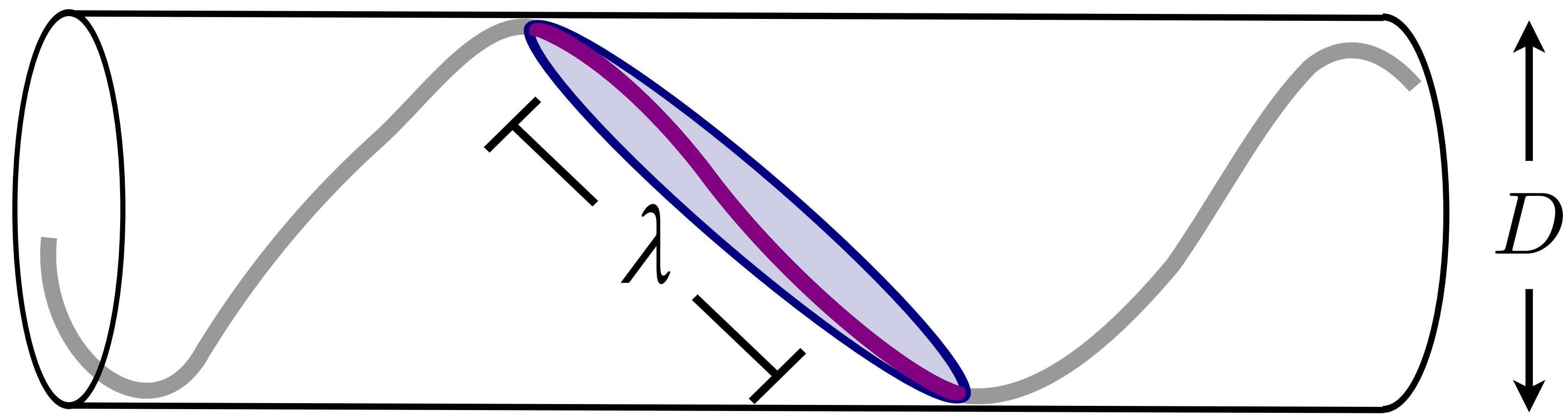


Tree et al. Macromolecules. (2013)
Chen and Noolandi. J. Chem. Phys. (1992)

Confined Chains

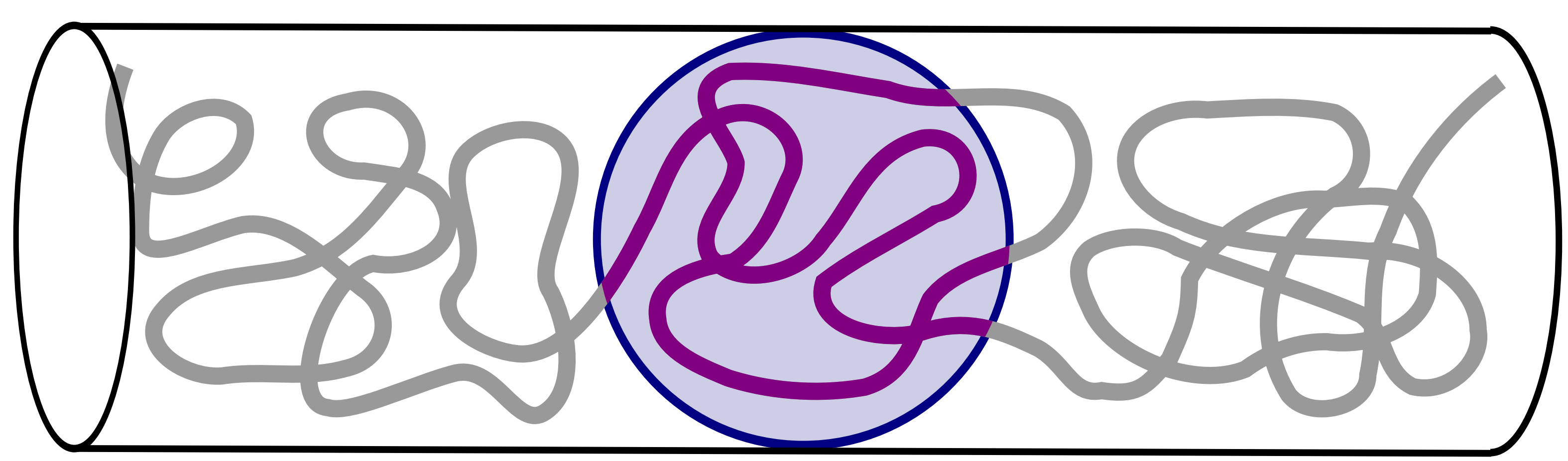
Bending Dominates

$$D \ll l_p$$



EV Dominates

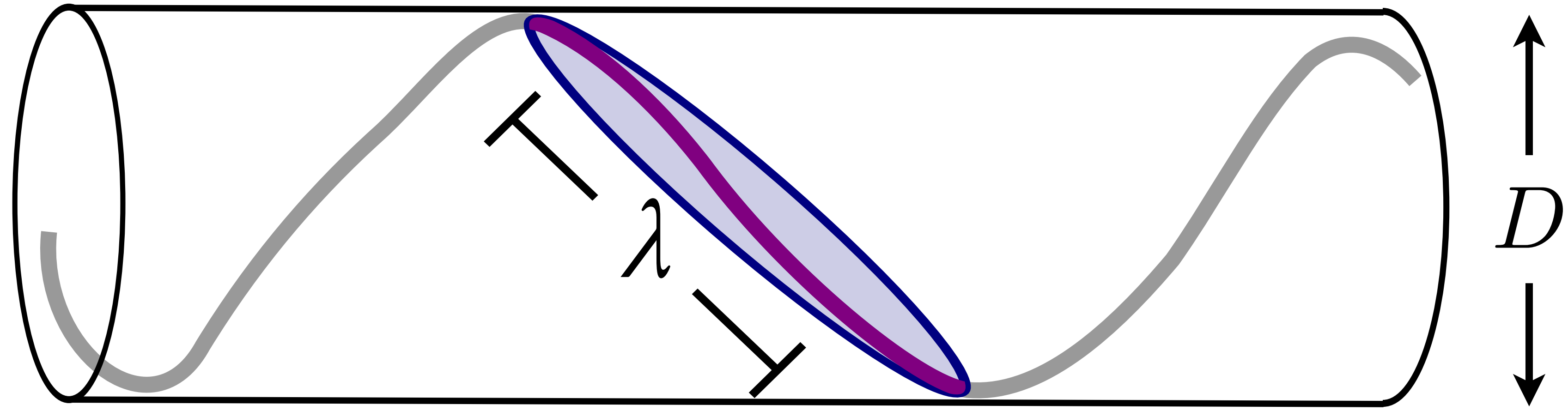
$$l_p^2/w \ll D \ll R$$

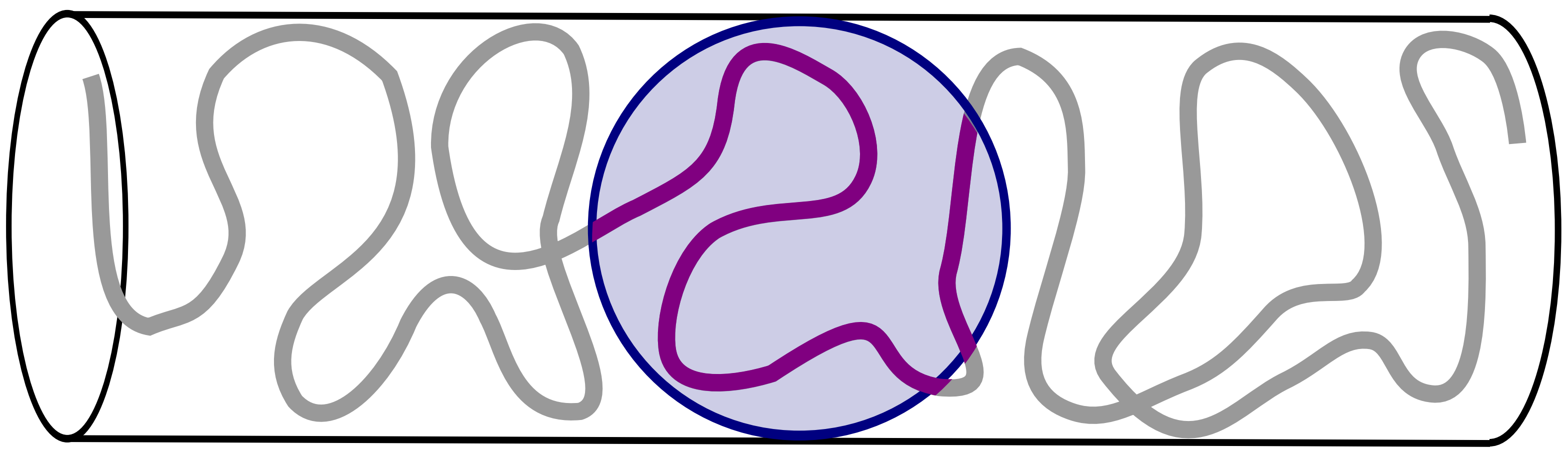


Confined Chains

Bending Dominates

$D \ll l_p$



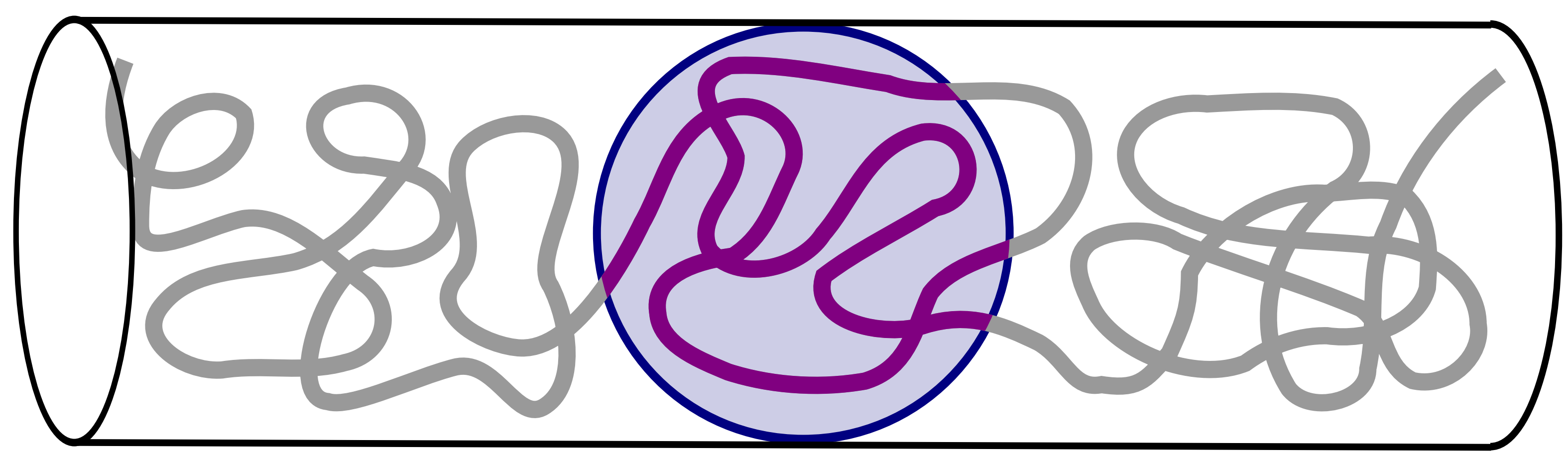


Weak EV

$l_p \ll D \ll l_p^2/w$

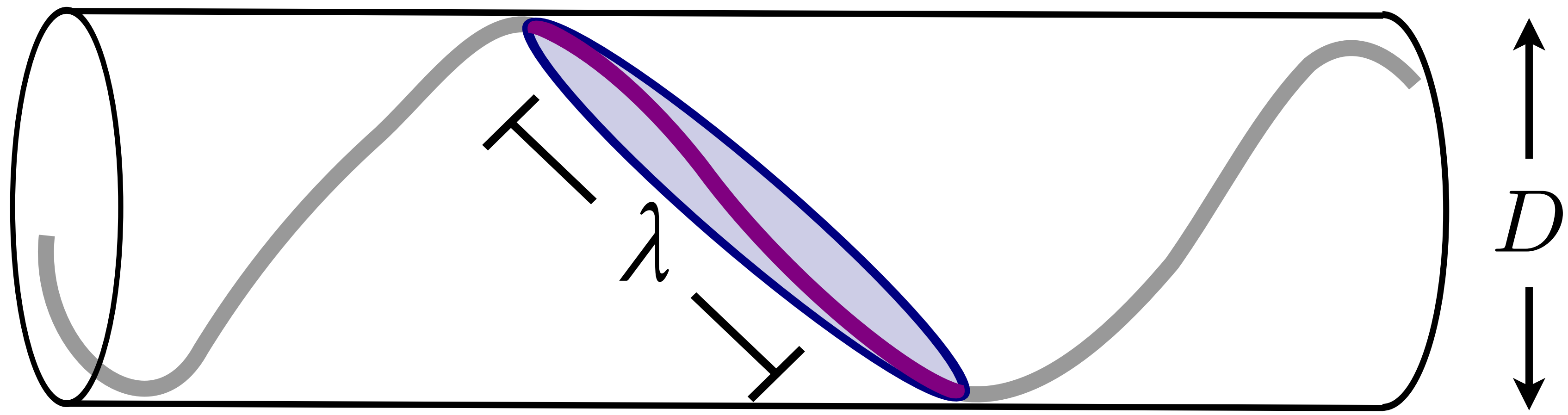
EV Dominates

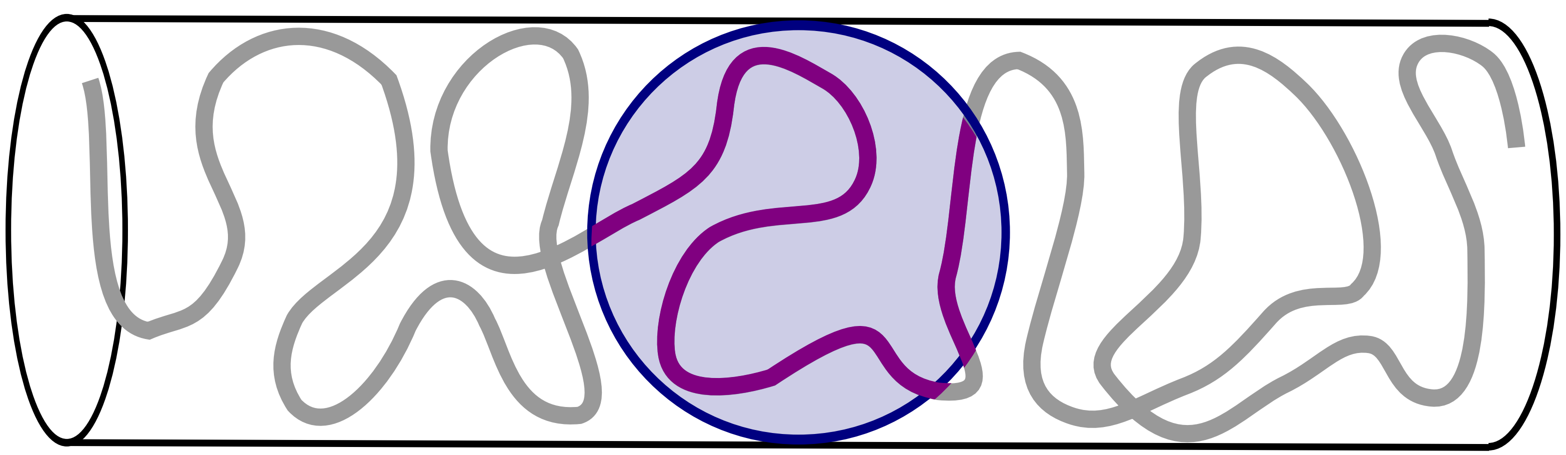
$l_p^2/w \ll D \ll R$



Confined Chains

$$F \sim F_0 D^{4/3}$$

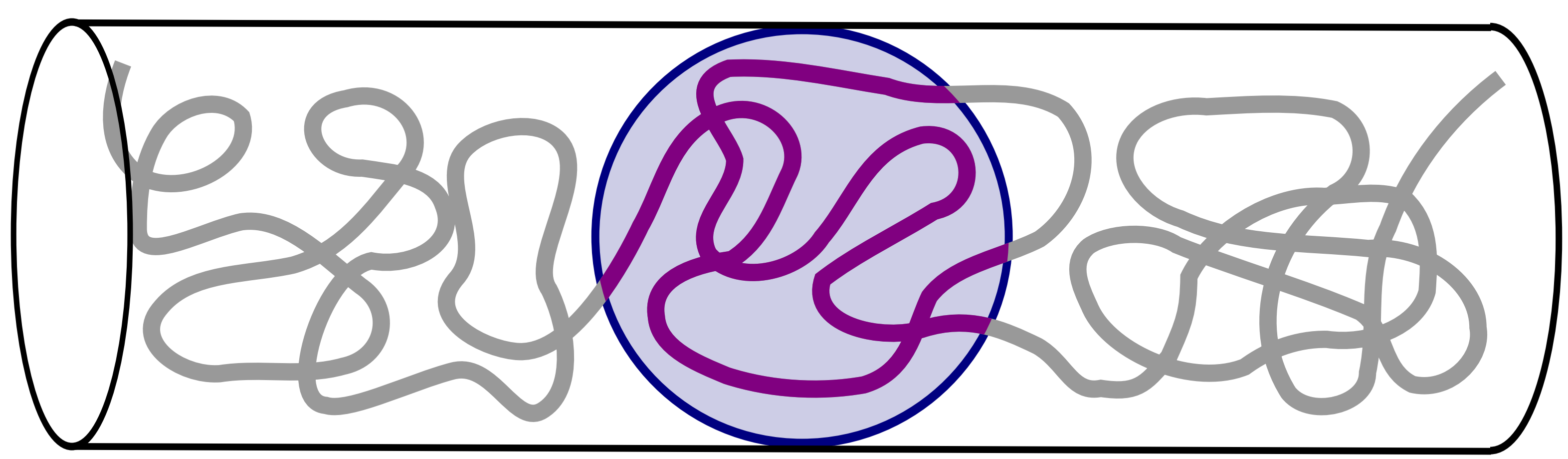




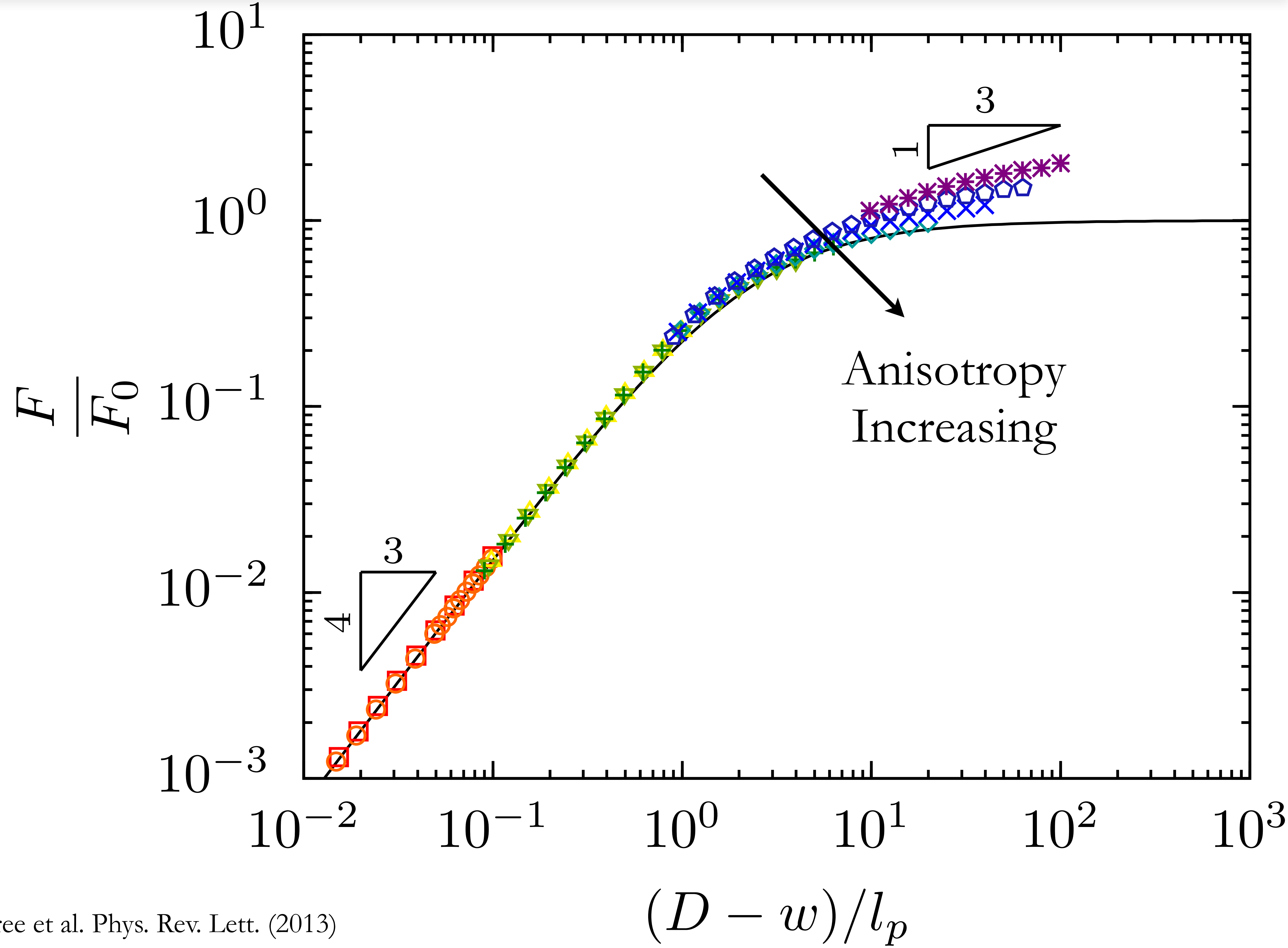
$$F \sim F_0$$

$$\sim k_B T L D^{-2}$$

$$F \sim F_0 D^{1/3}$$



Free Energy of Confinement

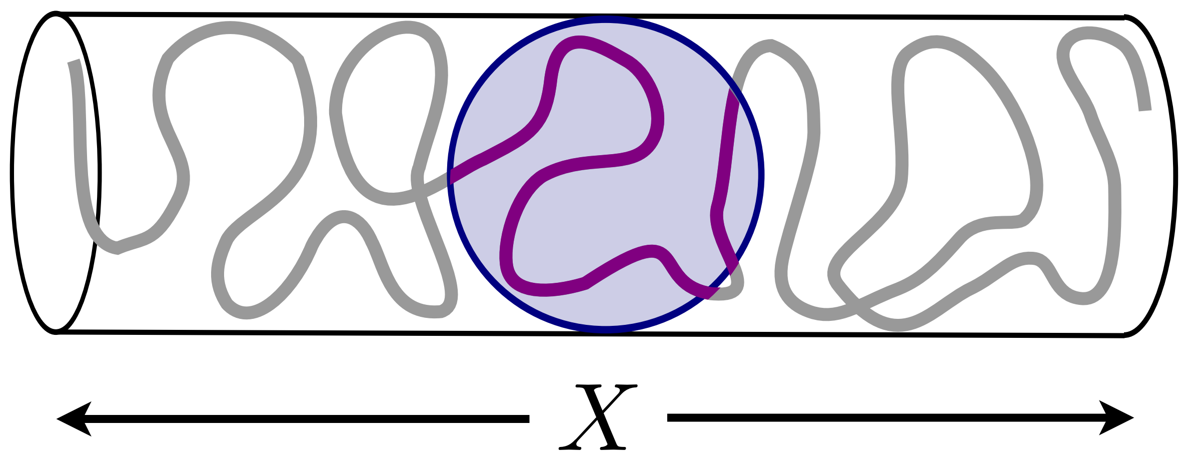


Tree et al. Phys. Rev. Lett. (2013)

Application to DNA

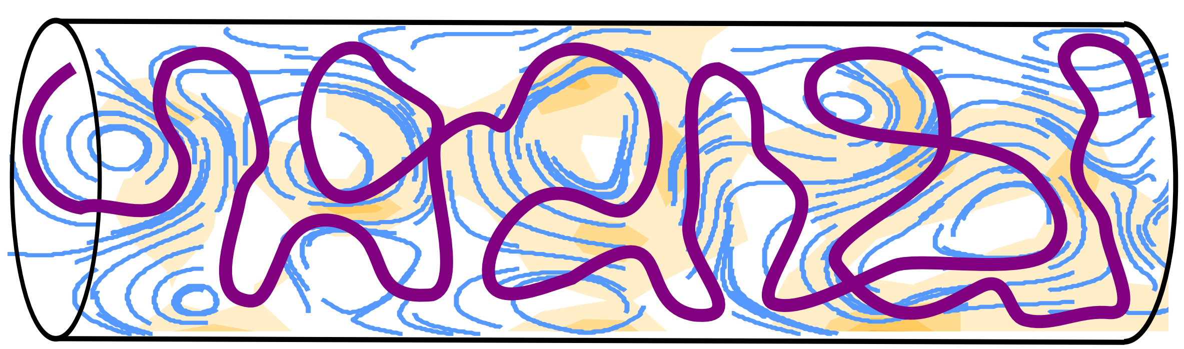
- Using this approach we can calculate and understand relevant properties for DNA mapping devices.

Mean Extension



Tree et al. Phys. Rev. Lett. (2013)
Wang et al. Macrmolecules (2011)

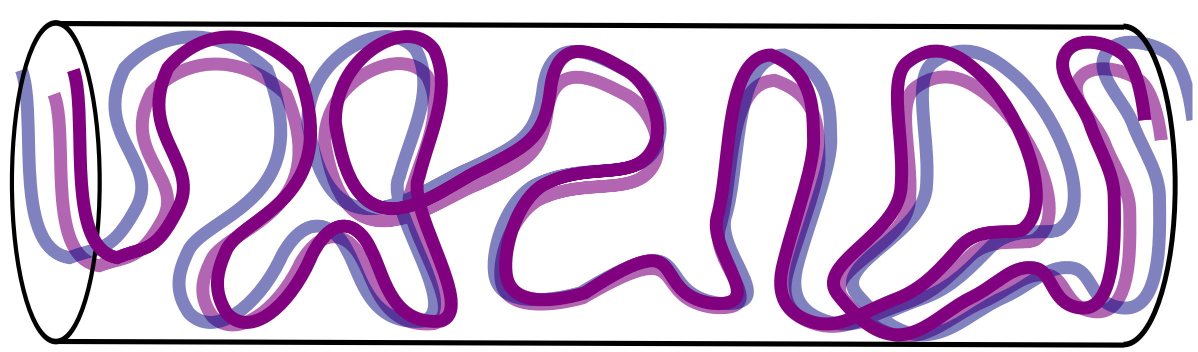
Diffusion/ Mobility



$$\mu = \mathcal{D}/k_B T \approx \langle \mathbf{\Omega}_{xx} \rangle$$

Tree et al. Phys. Rev. Lett. (2012)

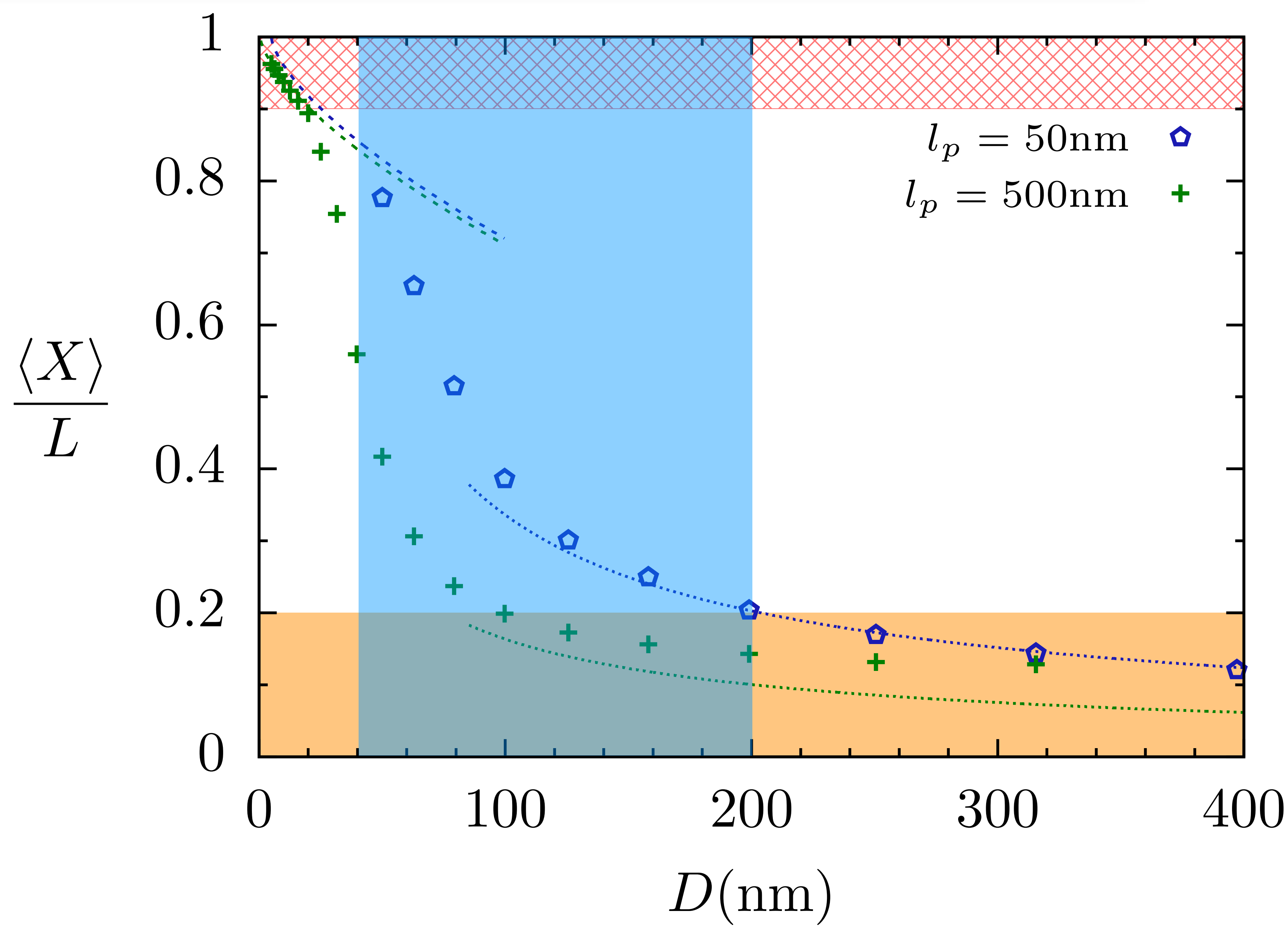
Fluctuations & Relaxation Time



$$\tau \sim \langle {\delta_X}^2 \rangle / \mu$$

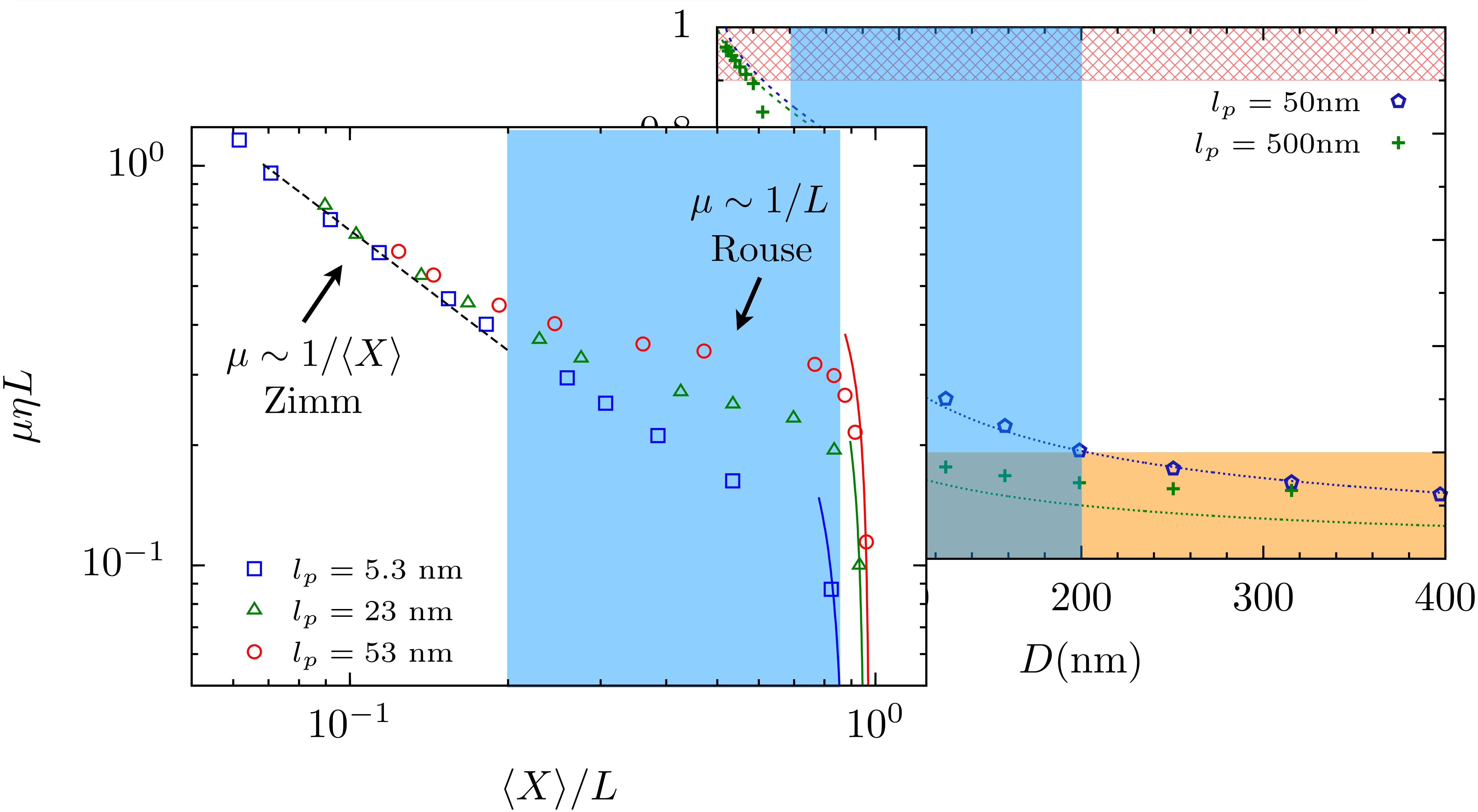
Tree et al. Biomicrofluidics (2013)

DNA in Nanochannels



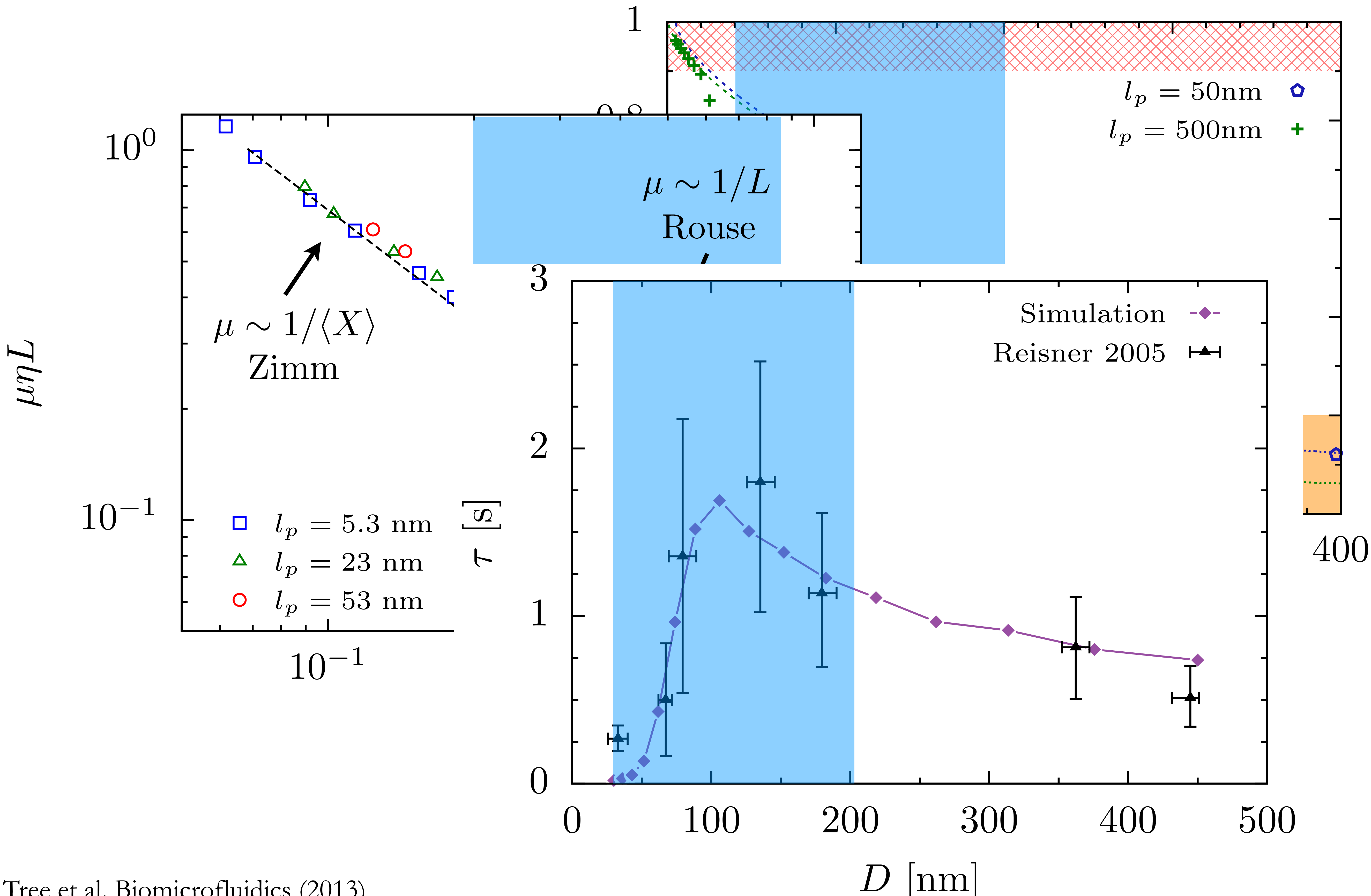
Tree et al. Phys. Rev. Lett. (2013)

DNA in Nanochannels



Tree et al. Phys. Rev. Lett. (2012)

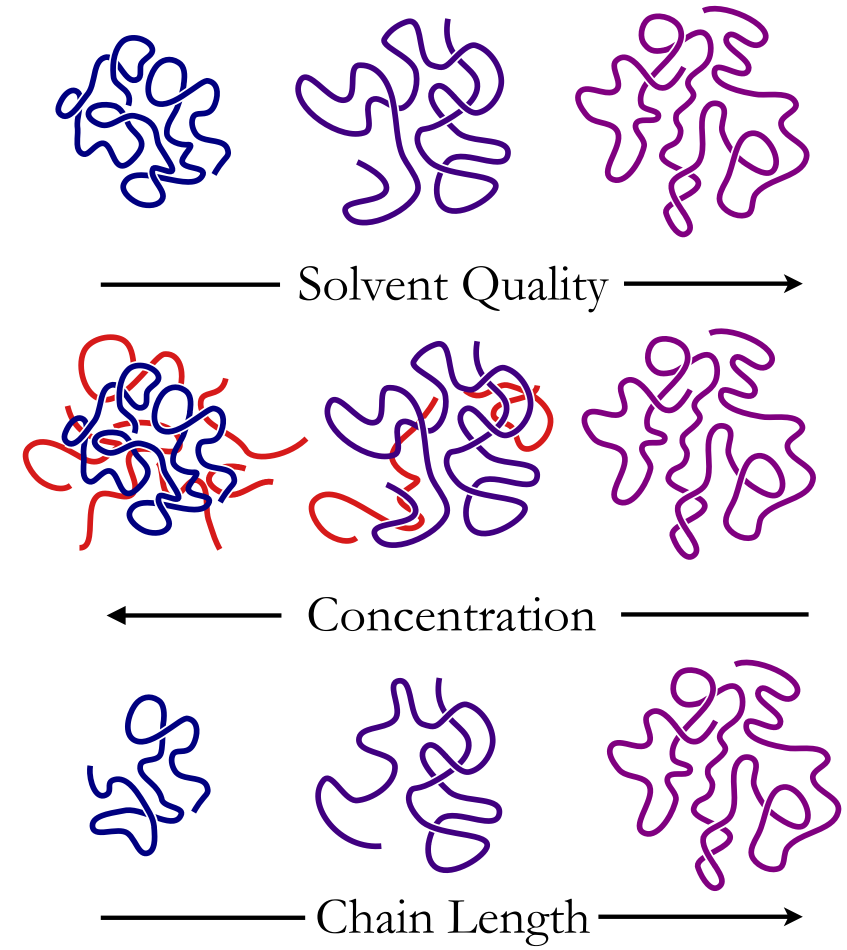
DNA in Nanochannels

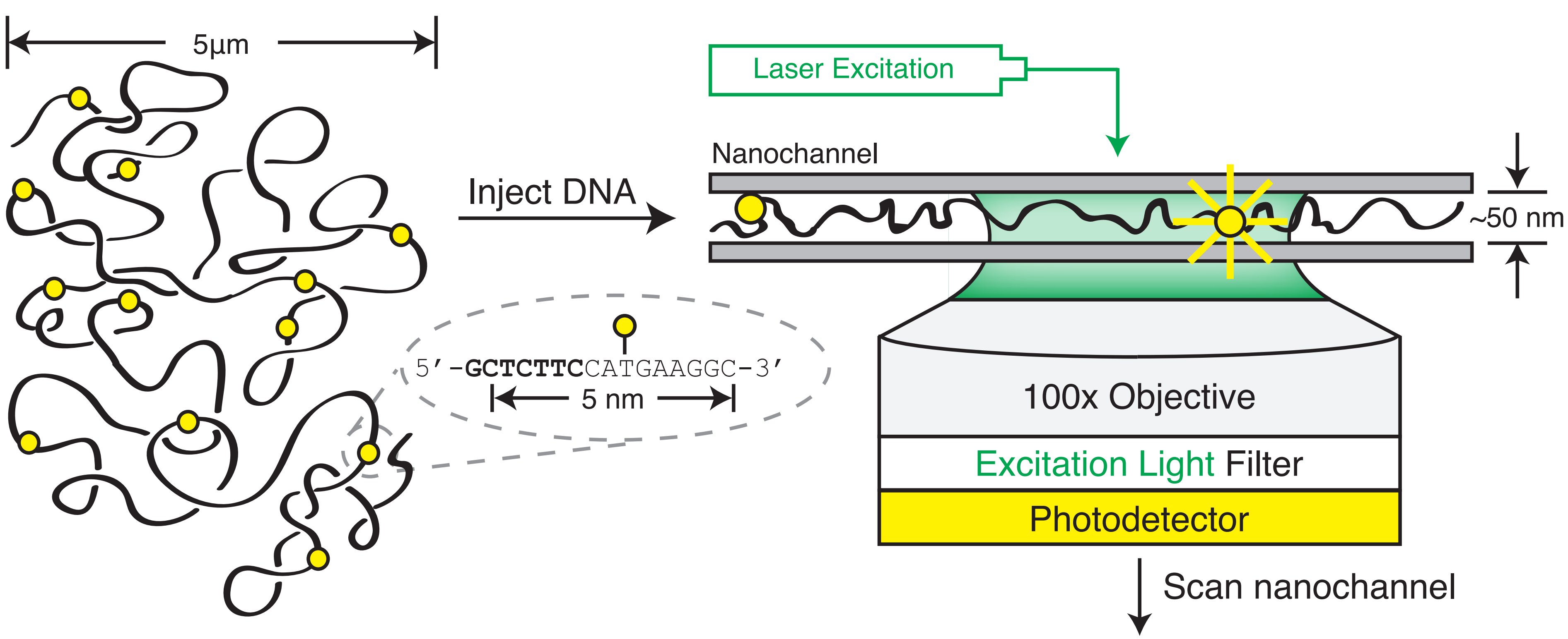


Tree et al. Biomicrofluidics (2013)

Conclusion

- Genomic mapping is a modern application of the excluded volume problem for the confined biopolymer, DNA.
  - The crossover depends on the monomer anisotropy of the chain.
  - Properties relevant to genomic mapping can be obtained by advanced Monte Carlo techniques (i.e. PERM).





Acknowledgments

Yanwei Wang

Tree, D., Wang, Y., Dorfman, K. Phys. Rev. Lett. (2012). Doi: 101103/PhysRevLett.108.228105

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Tree, D., Muralidhar, A., Doyle, P., Dorfman, K. Macromolecules. (2013). Doi: 10.1021/ma401507f

Tree, D., Wang, Y., Dorfman, K. Biomicrofluidics. (2013). Doi: 10.1063/1.4826156

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