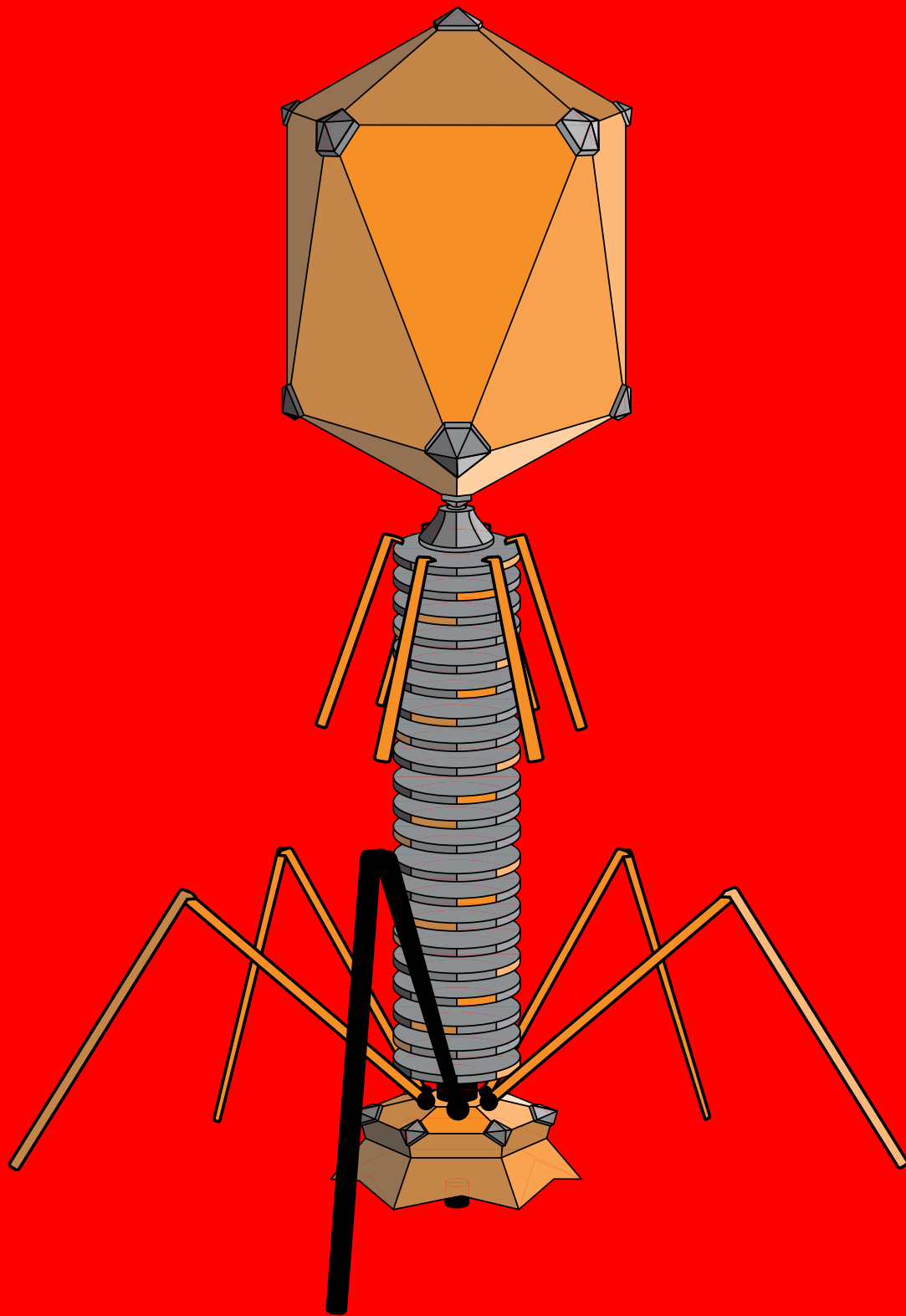
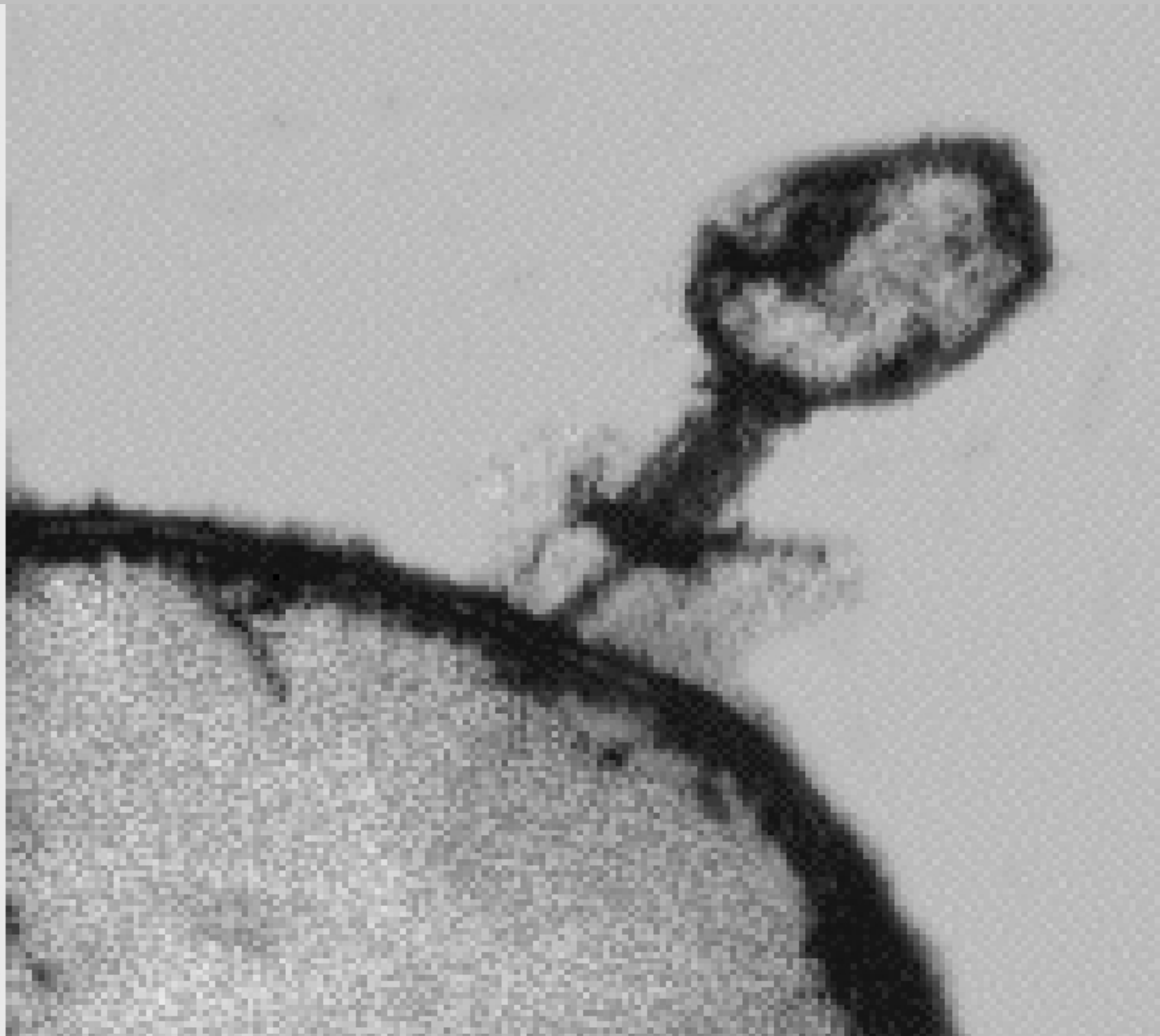
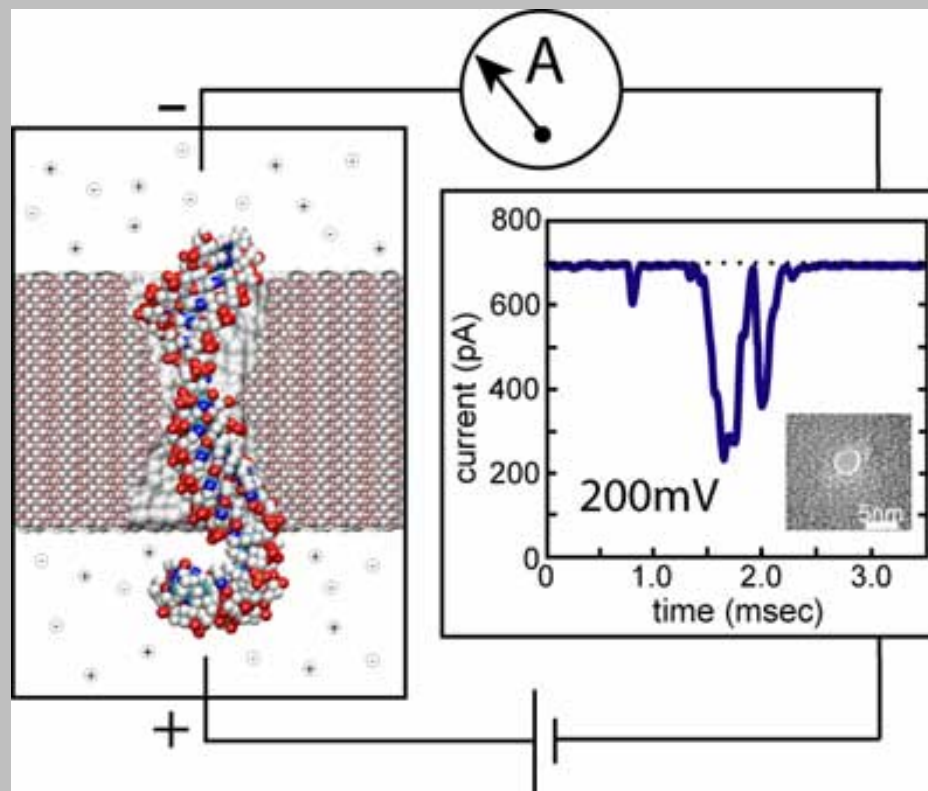
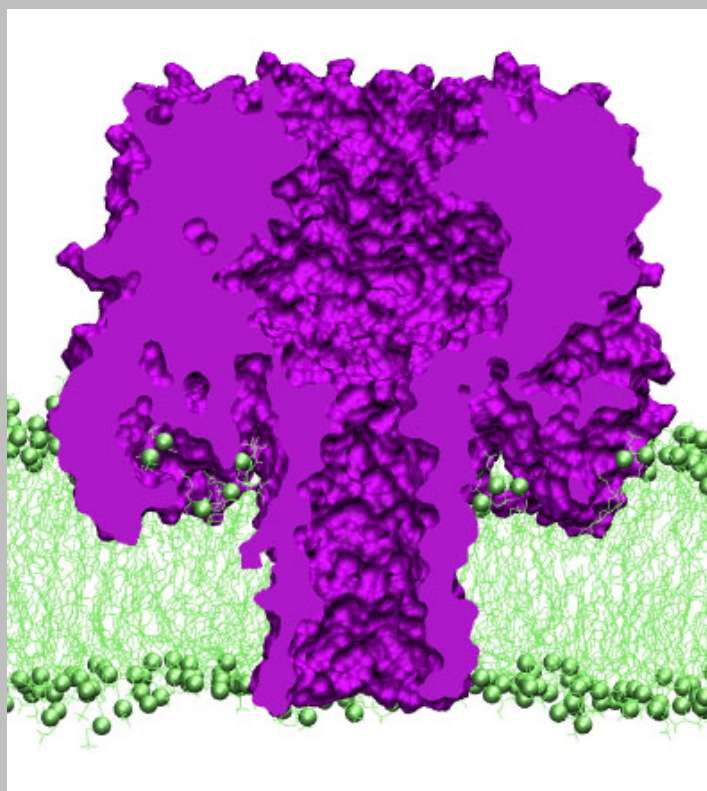
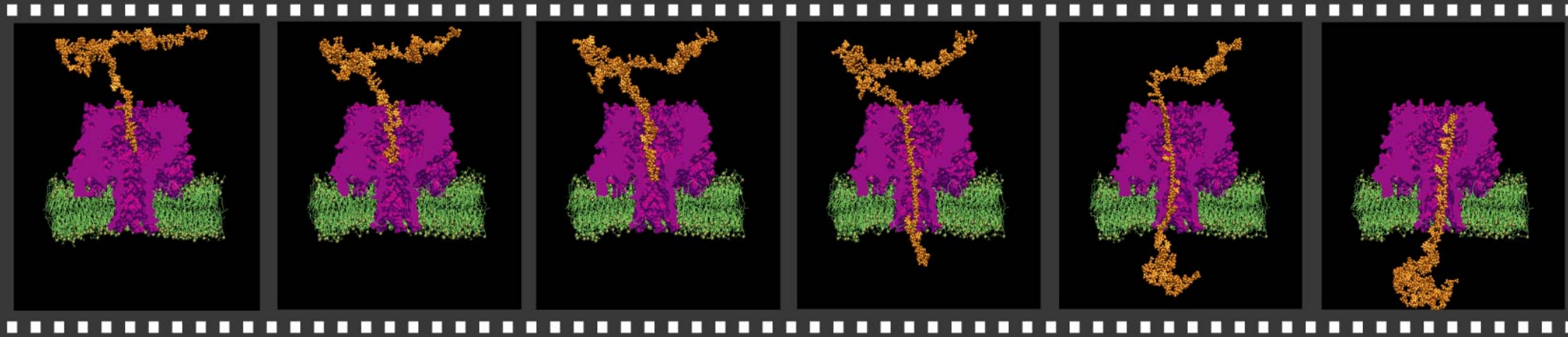
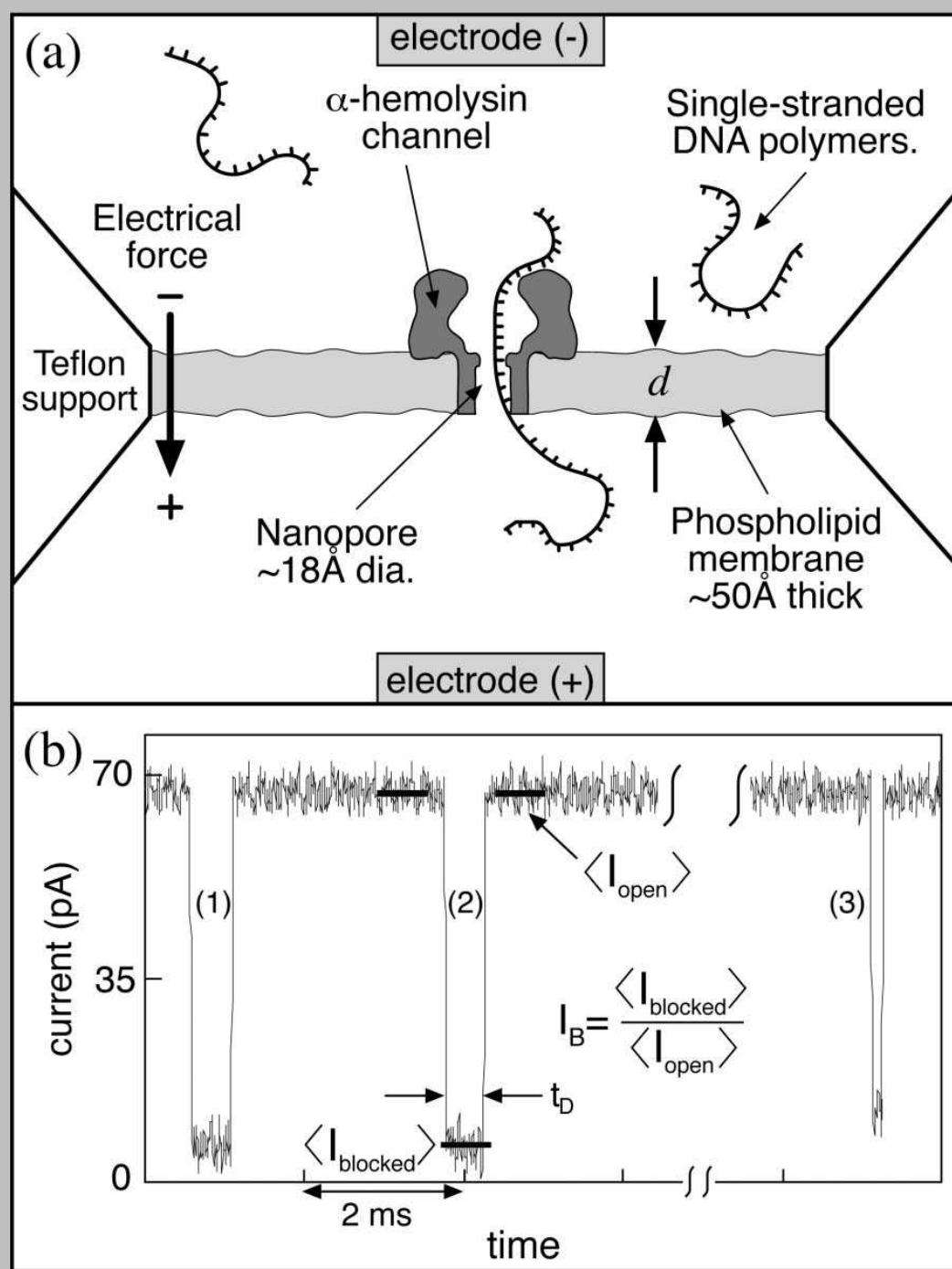


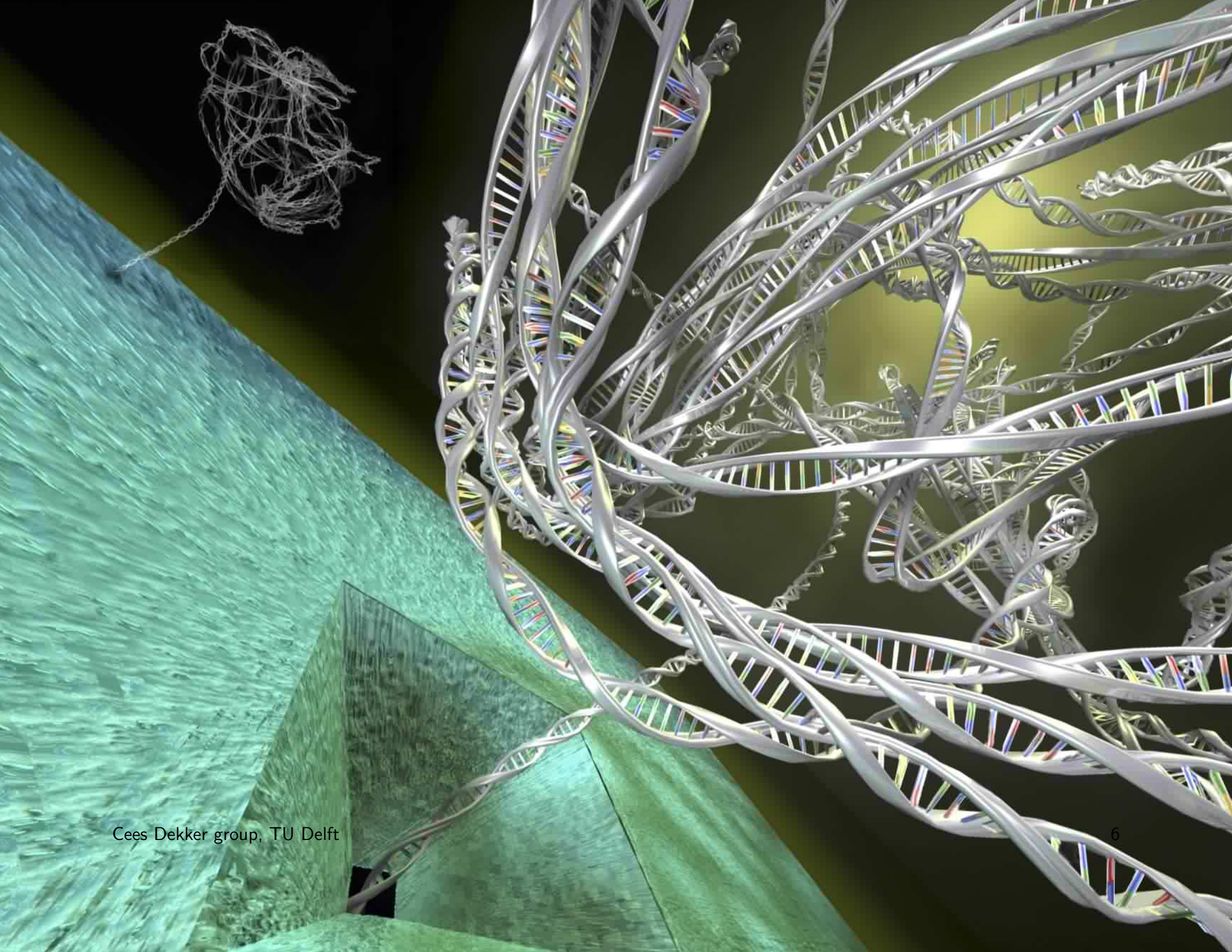
Polymer translocation through nanopores







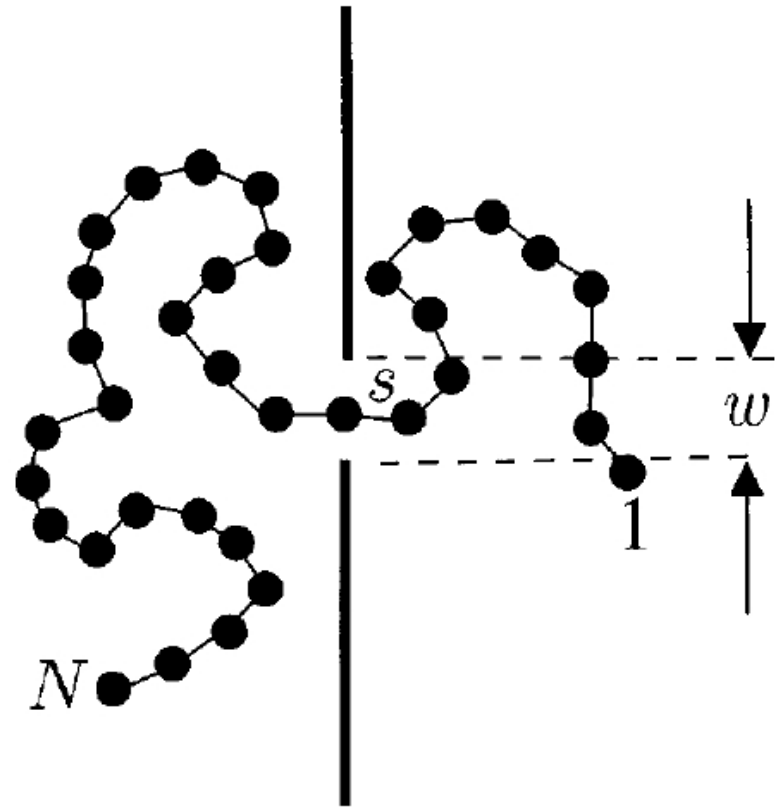




Polymer model for translocation

1. Chain is polymer with N monomers
2. Chain is already threaded into pore
3. Reflecting B.C. @ $s = 0$
4. Absorbing B.C. @ $s = N$
5. Neglect chain-pore interactions
6. \exists reaction coordinate:

$$s = \# \left\{ \begin{array}{l} \text{translocated} \\ \text{monomers} \end{array} \right\}$$



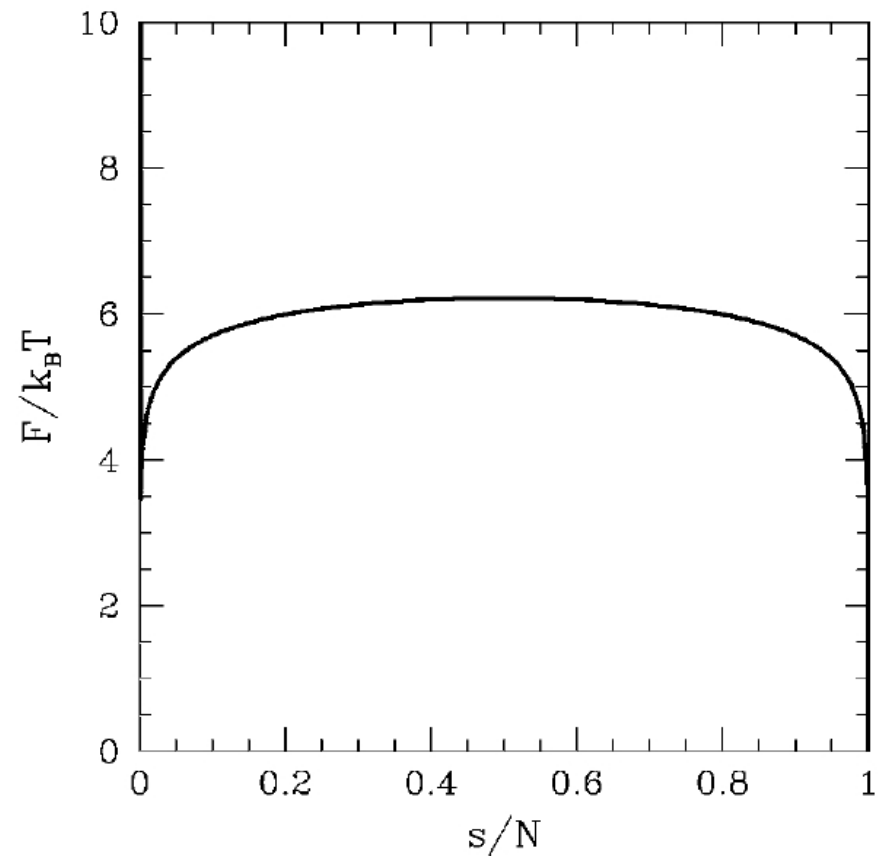
Entropic barrier

d.o.f. of a chain with N monomers:

$$\omega \simeq \mu^N N^{\gamma_g - 1}$$

s -dependence of free energy

$$\mathcal{F}(s) \simeq (\gamma_g - 1)k_B T \log([N - s]s)$$

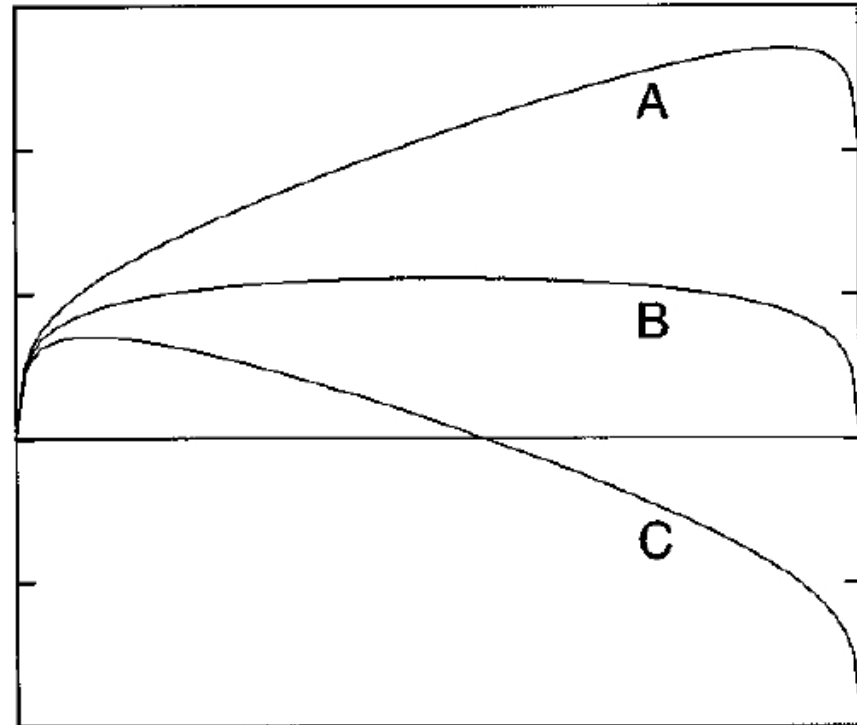


\rightsquigarrow driving force needed for efficient translocation

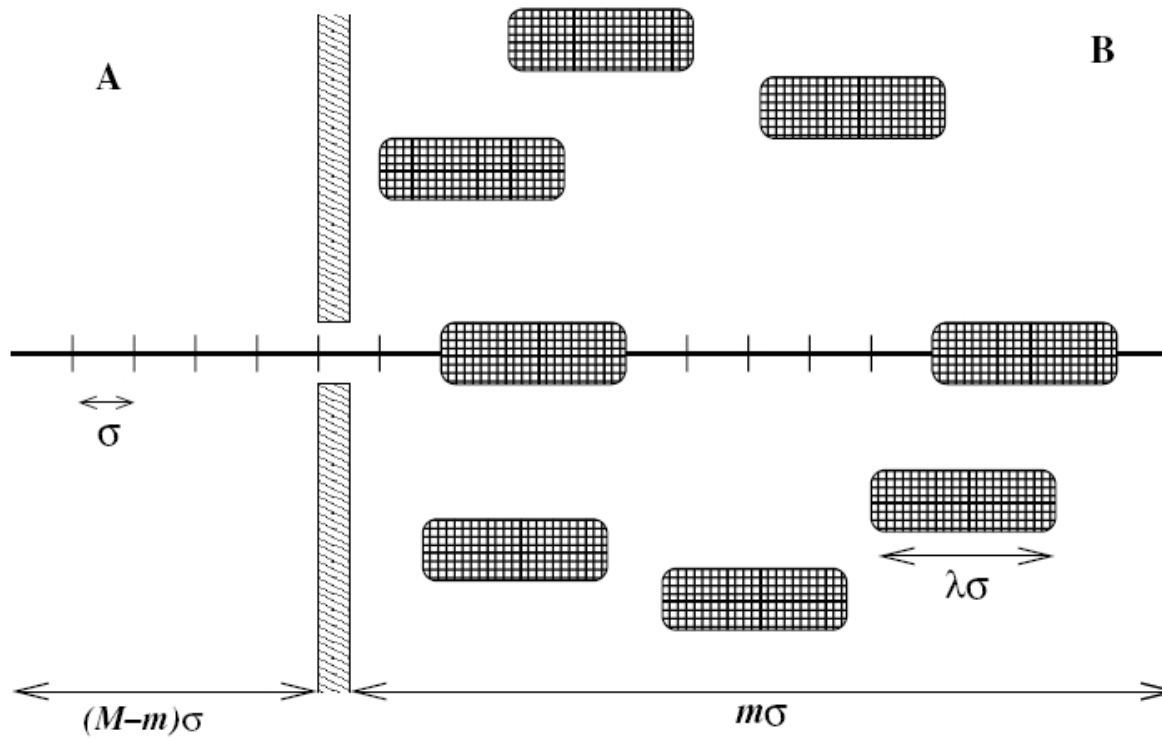
Driving force

Driving force creates chemical potential difference $\Delta\mu$ per monomer \rightsquigarrow drift

1. Trans-membrane potential
2. Binding proteins
3. Cis confinement (e.g., virus)
4. Active pulling

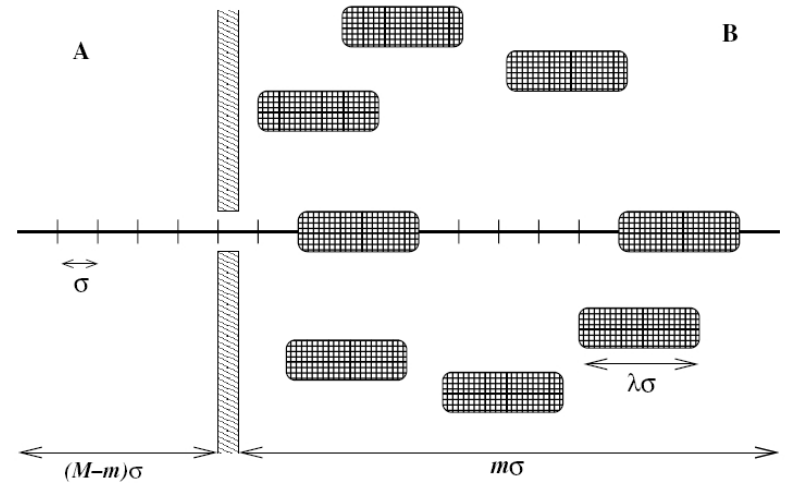


Chaperone-driven translocation



Chaperone-driven translocation

Driving: neglect polymeric d.o.f.

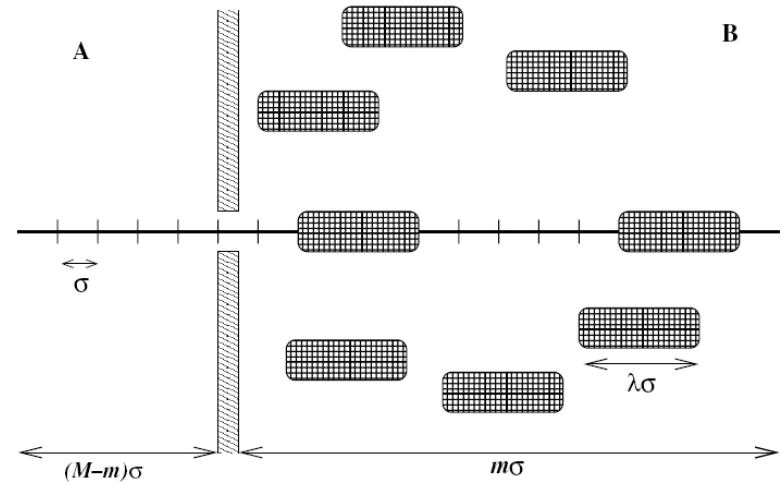


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Forward translocation rate:

$$t^+(m, n) = k$$



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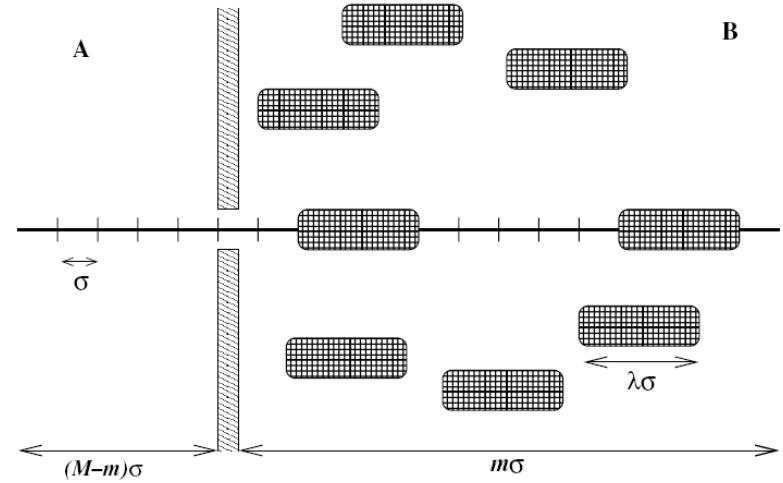
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Backward translocation rate:

$$t^-(m, n) = k \times \Pr \left\{ \begin{array}{l} \text{trans binding site} \\ \text{site closest to} \\ \text{pore is vacant} \end{array} \right\}$$



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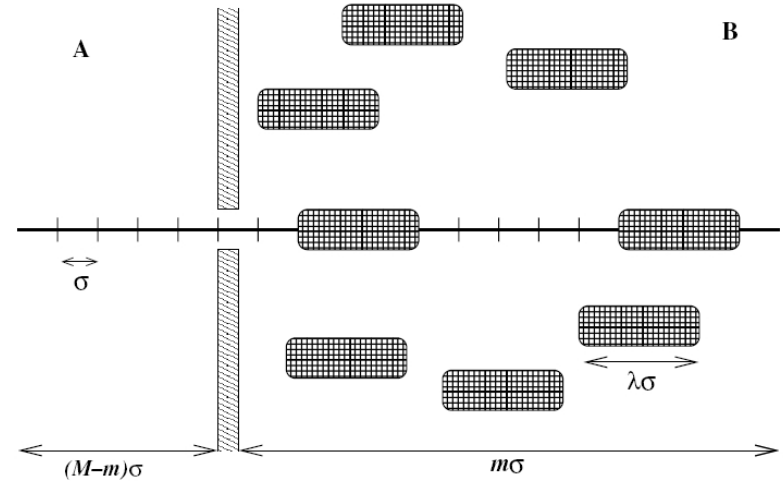
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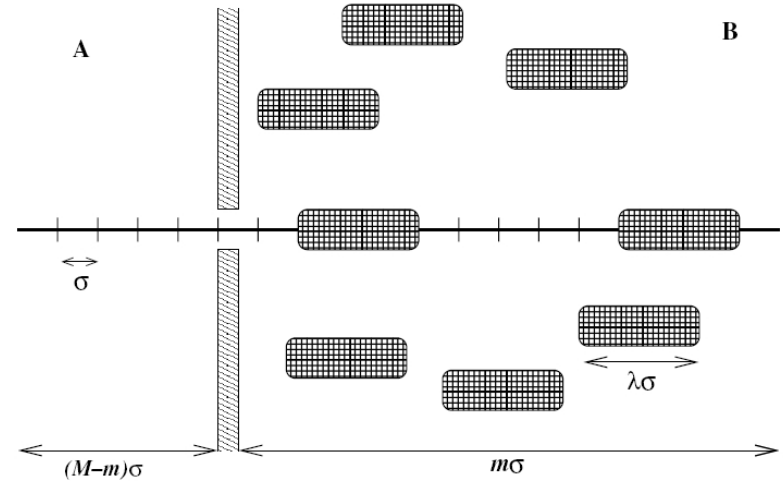
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Chaperone binding rate:

$$r^+(m, n) = c_0 K^{\text{eq}} \times \mathcal{N} \left\{ \begin{array}{l} \text{ways to add addtl} \\ \text{chaperone if} \\ n \text{ bound already} \end{array} \right\}$$

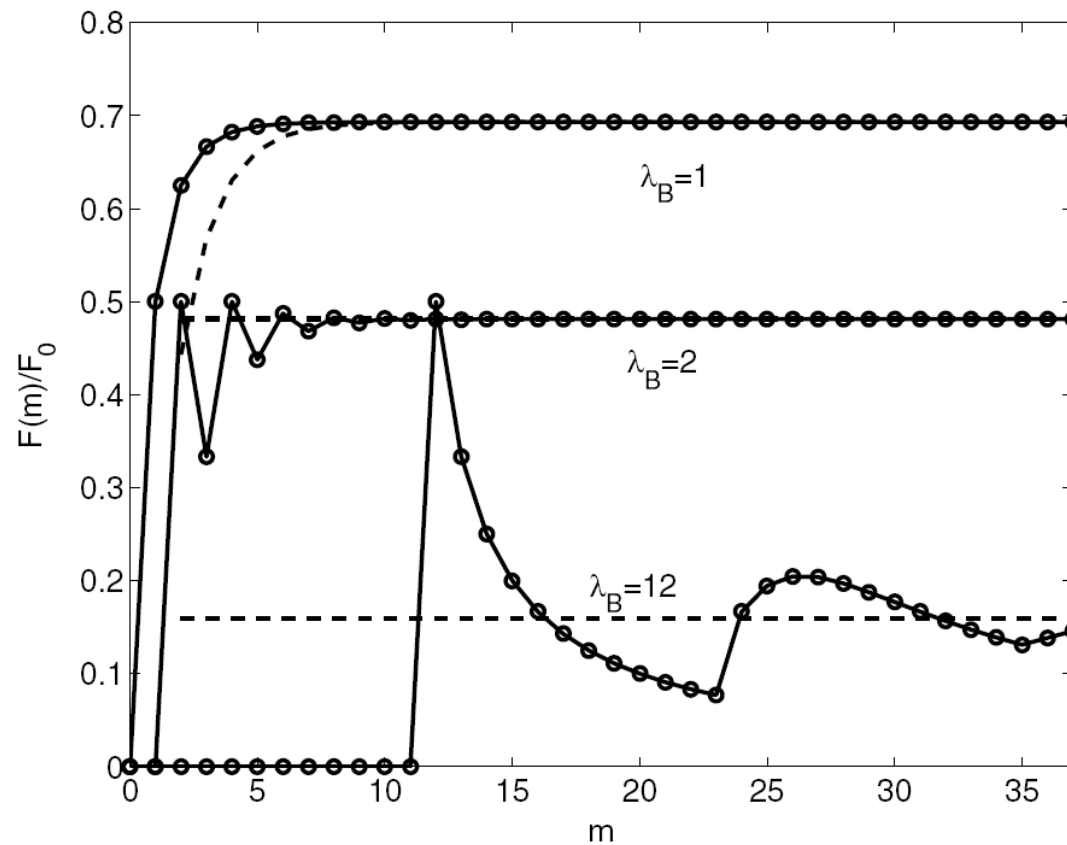


Chaperone-driven translocation

1. Slow binding dynamics: purely diffusive motion $\tau_T \simeq N^2$
2. Slow unbinding dynamics: ratcheted motion $\tau_T \simeq N$
3. Fast binding/unbinding: adiabatic elimination of chaperone dynamics

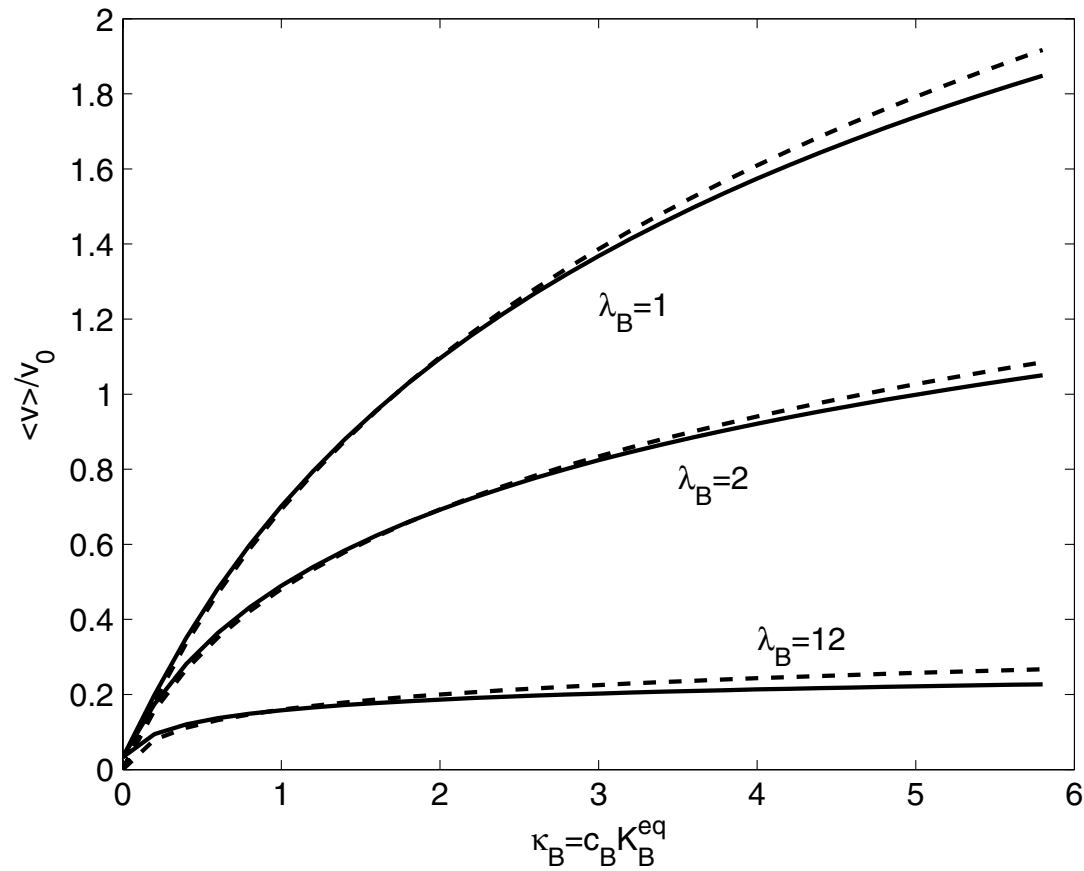
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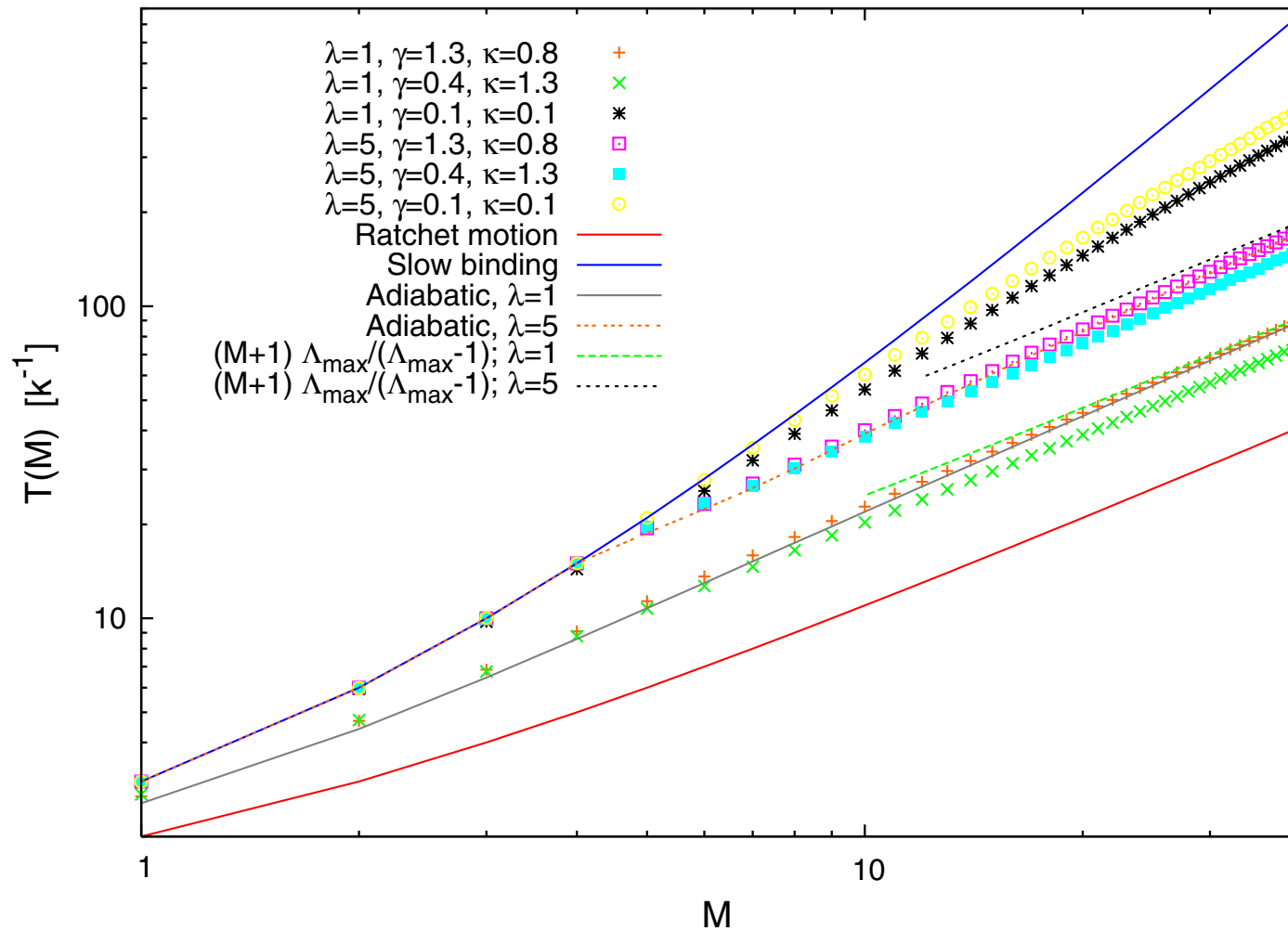
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Dependence of mean translocation velocity on binding strength:



Chaperone-driven translocation

Mean translocation time as function of chain length:



Polymer translocation: many groups, many opinions ...



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Translocation dynamics sufficiently slow \rightsquigarrow diffusion in potential with PDF $P(s, t)$

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NB: For s -independent drift: $\tau_T \simeq N/V$ where V the stationary velocity

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SA chain ($\nu(2D) = 3/4$ and $\nu(3D) = 0.59$): τ_R longer than translocation time τ_T **f**

Non-Brownian translocation dynamics

Extended simulations in 1D: $\tau_T \simeq N^2$

In 2D: $\tau_T \simeq N^{2.5}$

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6. $\rightsquigarrow \zeta(2D) = 0.4$ and $\zeta(3D) \approx 0.46$, i.e., subdiffusion

Fractional approach to translocation dynamics

Pausing events of duration t distributed as

$$\psi(t) \simeq \frac{\tau^\alpha}{t^{1+\alpha}} \quad \therefore \quad \langle t \rangle = \int_0^\infty t\psi(t)dt \rightarrow \infty$$

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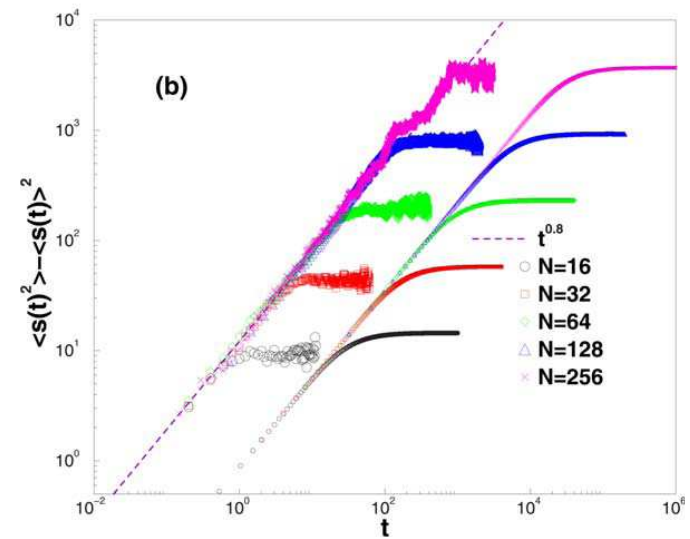
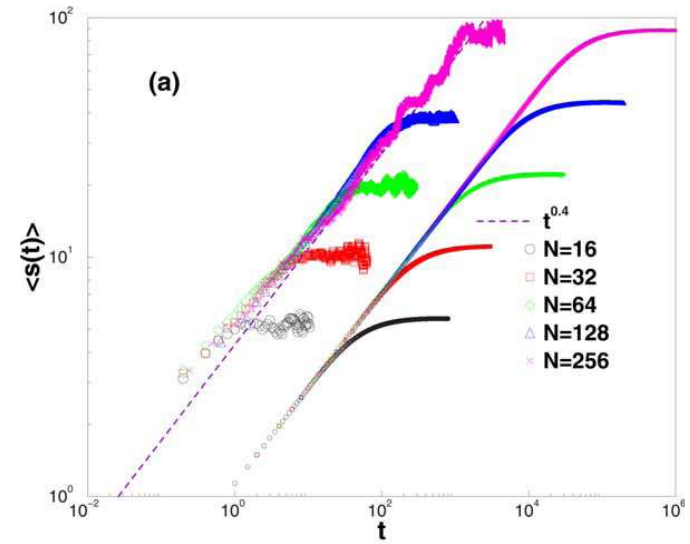
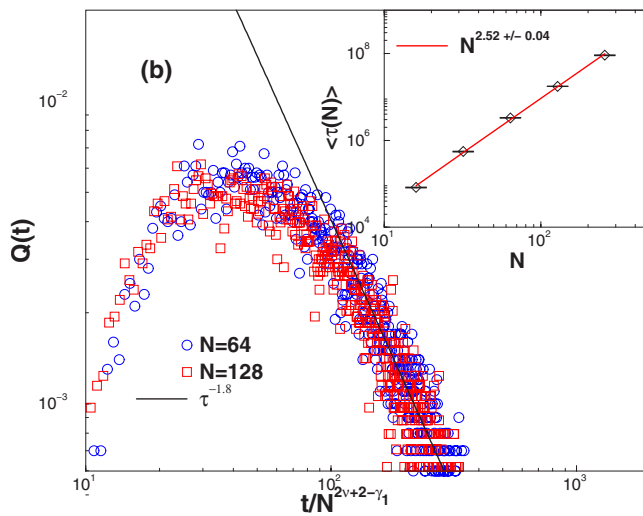
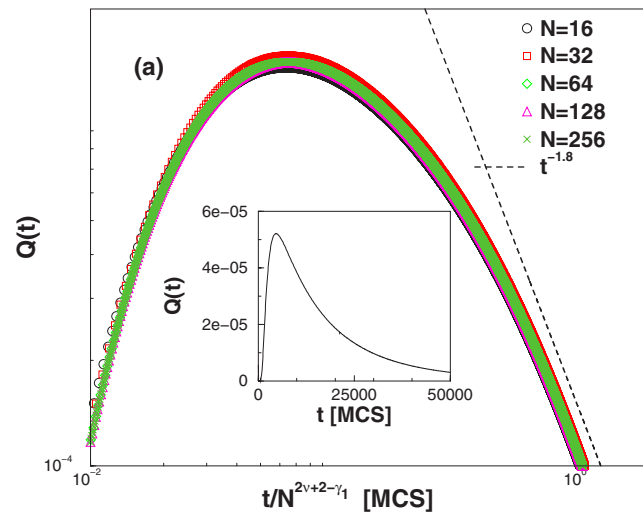
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Mode relaxation:

$$T_n(t) = t_n E_\alpha \left(-\lambda_{n,\alpha} t^\alpha \right) \sim t_n \begin{cases} 1 - t^\alpha / \Gamma(1 + \alpha) \\ t^{-\alpha} / \Gamma(1 - \alpha) \end{cases}$$

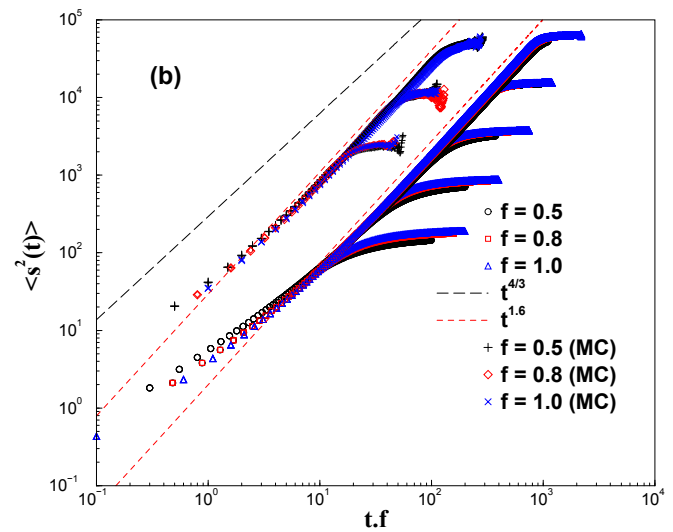
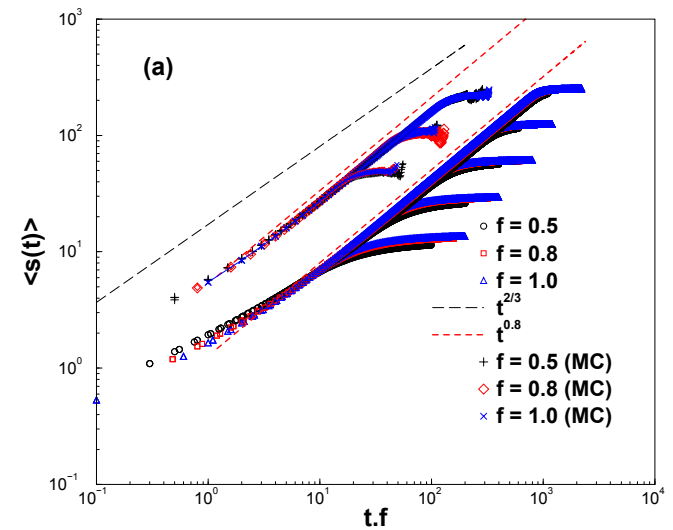
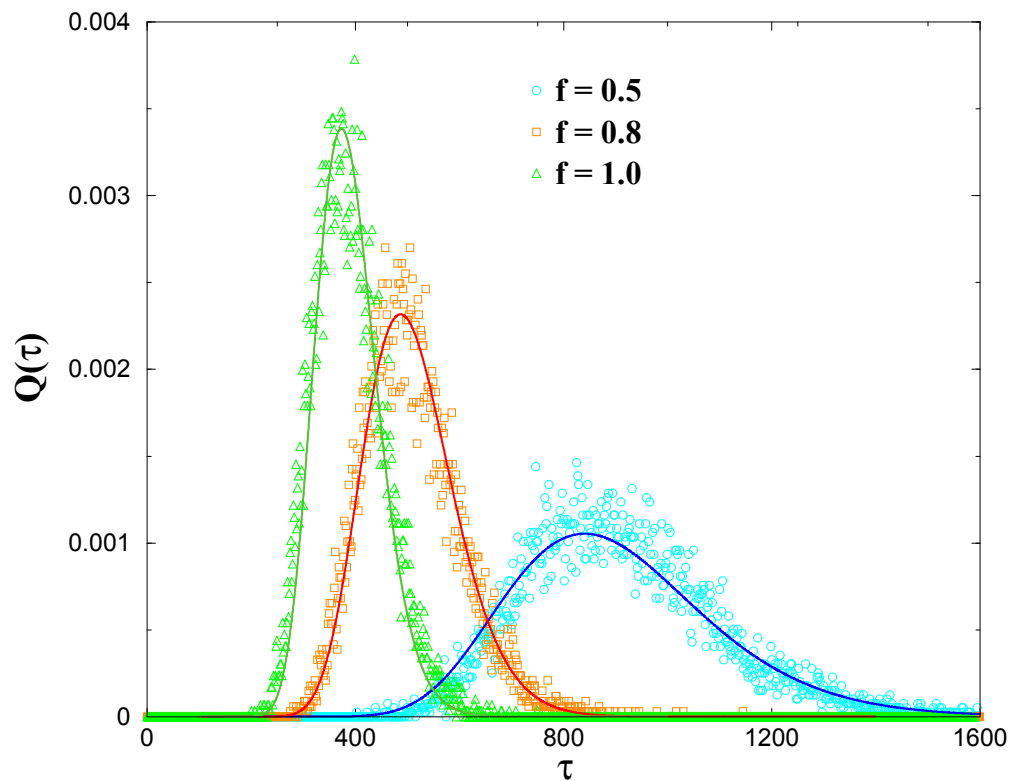
Agreement with simulations data: drift-free case

Theory prediction



Agreement with simulations data: constant drift case

First passage time distribution:



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REM: Rouse relaxation time $\tau_R \simeq N^{1+2\nu}$

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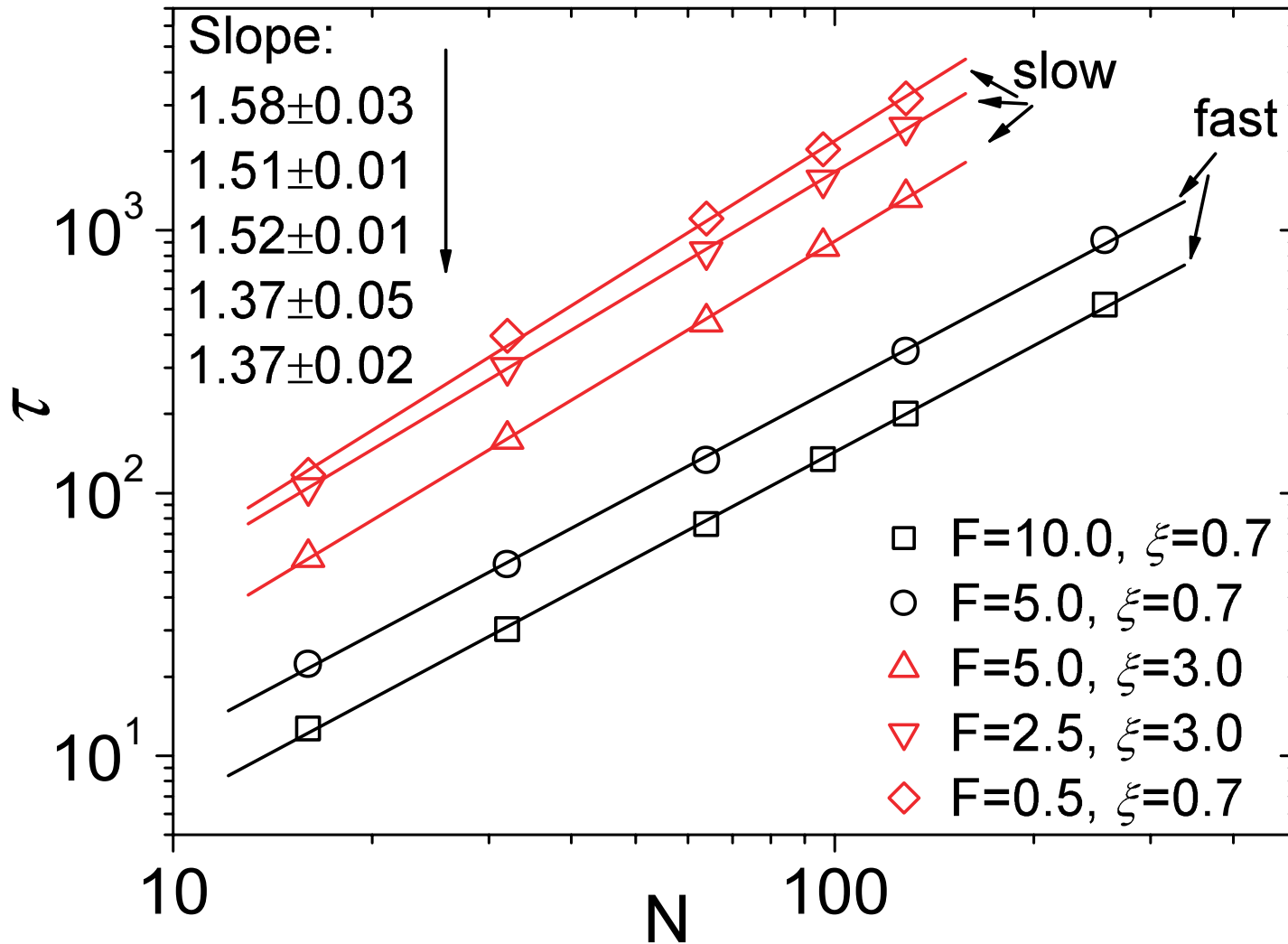
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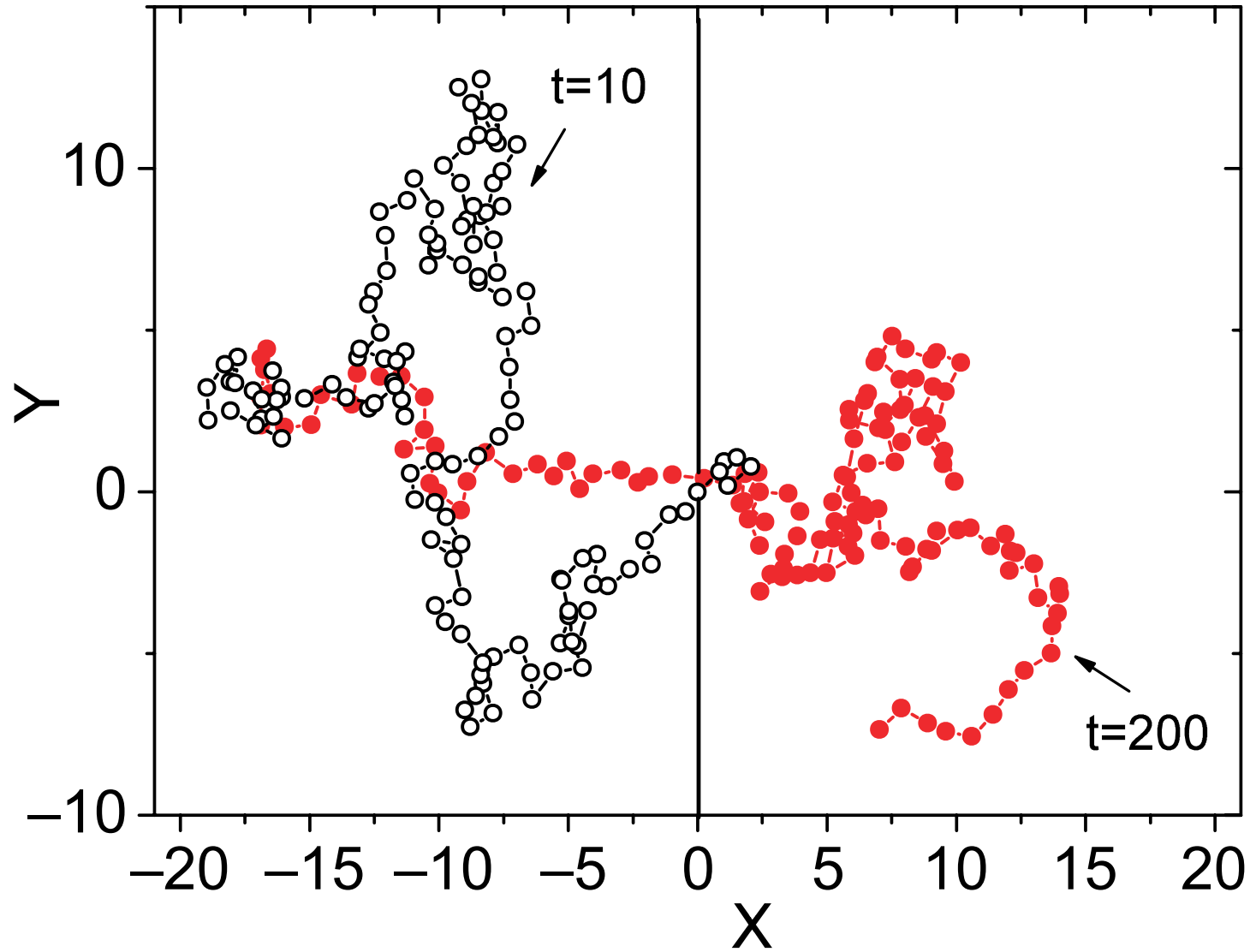
Yes, we can . . .

Slow versus fast translocation

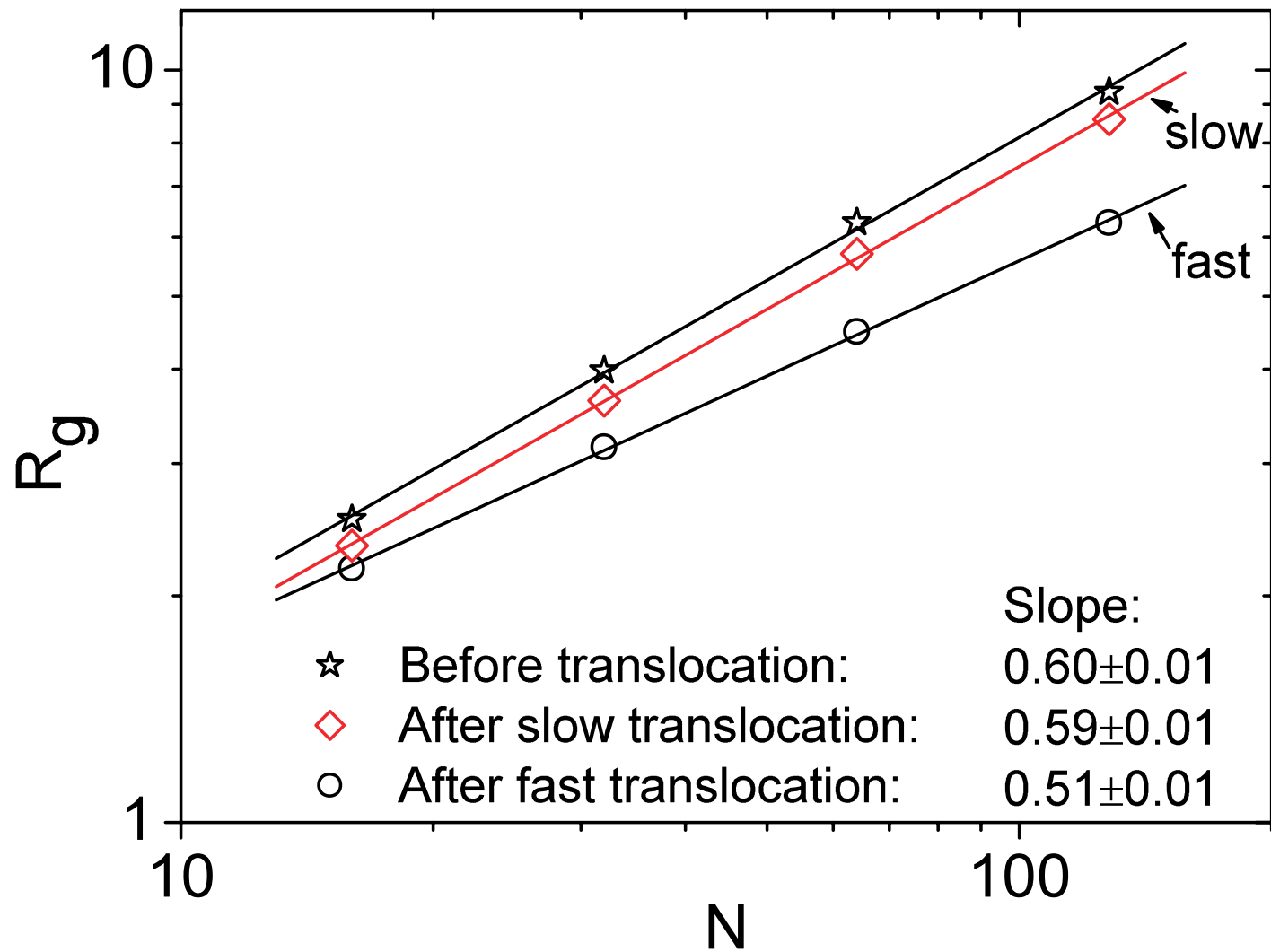


In 3D interpolation between $\alpha = 1 + \nu \approx 1.59$ and $\alpha' = (1 + 2\nu)/(1 + \nu) \approx 1.37$

Fast translocation: nonequilibrium effects

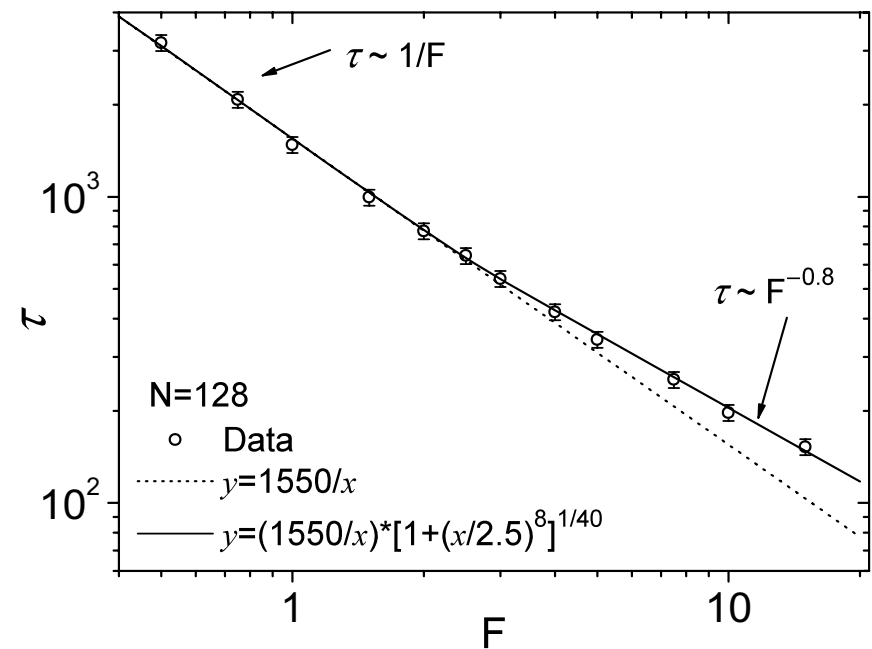
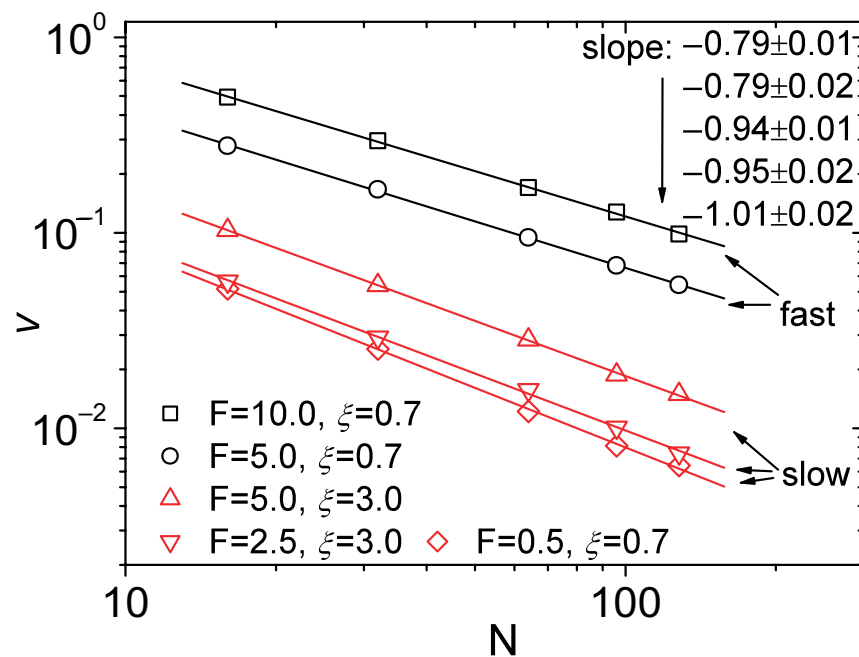


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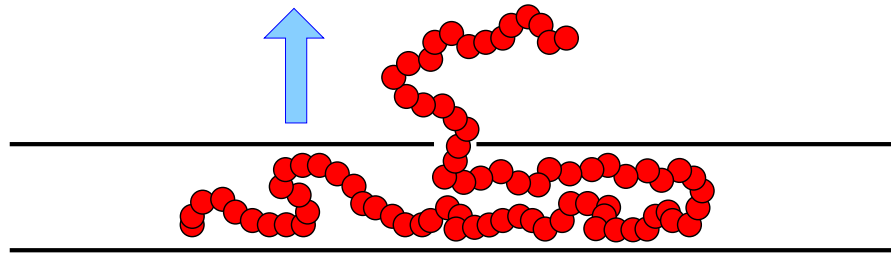


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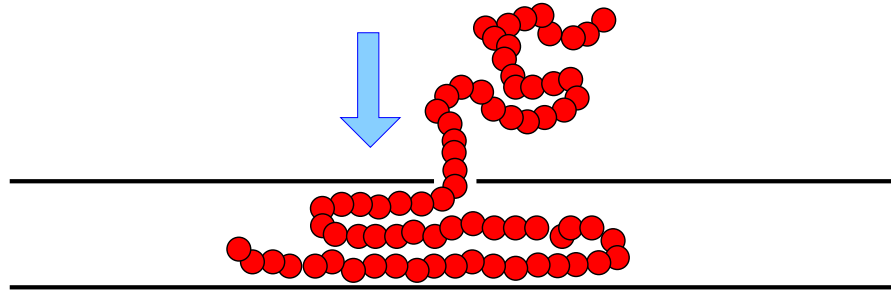
	F	ξ	F/ξ	$\alpha (\tau \sim N^\alpha)$	$\delta (v \sim N^\delta)$	$\beta (\langle s(t) \rangle \sim t^\beta)$	$\alpha\beta$
Fast	10.0	0.7	14.28	1.37 ± 0.02	-0.79 ± 0.01	0.84 ± 0.01	1.15
	5.0	0.7	7.14	1.37 ± 0.05	-0.79 ± 0.02	0.85 ± 0.01	1.16
Slow	5.0	3.0	1.67	1.52 ± 0.01	-0.94 ± 0.01	0.71 ± 0.01	1.08
	2.5	3.0	0.83	1.51 ± 0.02	-0.95 ± 0.02	0.69 ± 0.01	1.04
	0.5	0.7	0.71	1.58 ± 0.03	-1.01 ± 0.02	0.64 ± 0.01	1.01



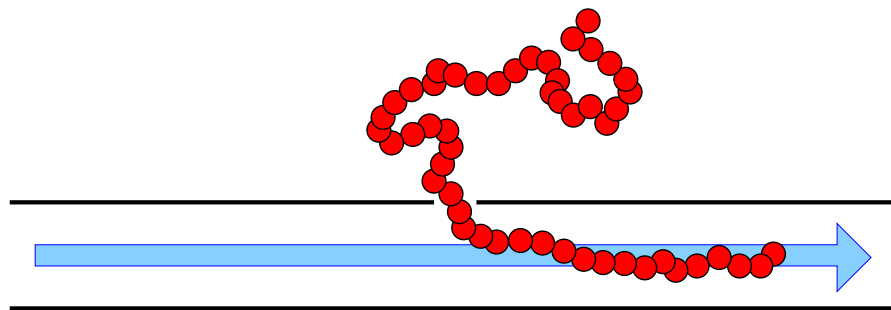
Variations on a theme



Out of confinement



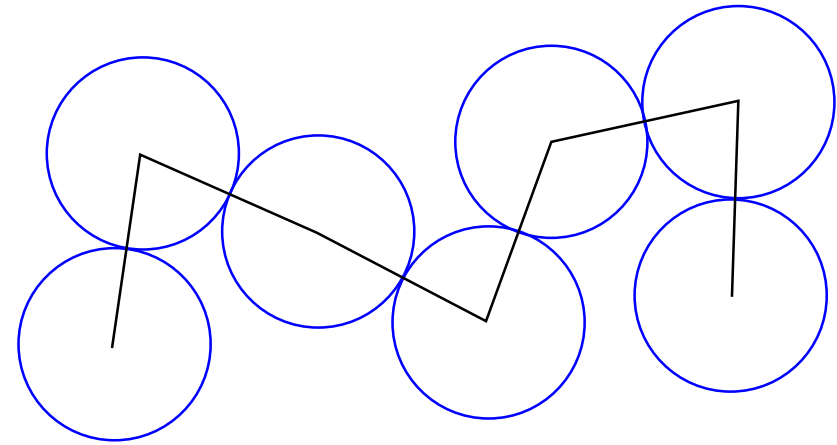
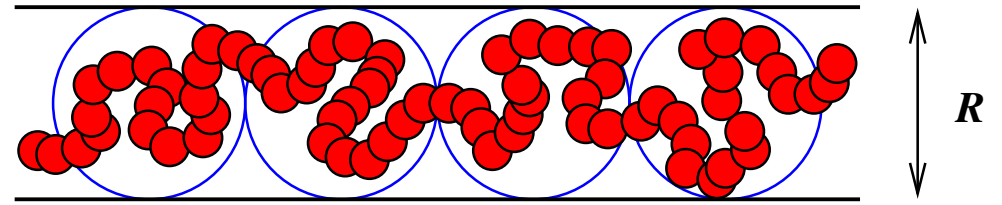
Into confinement



The chain sucker

Translocation into a laterally unbounded confinement

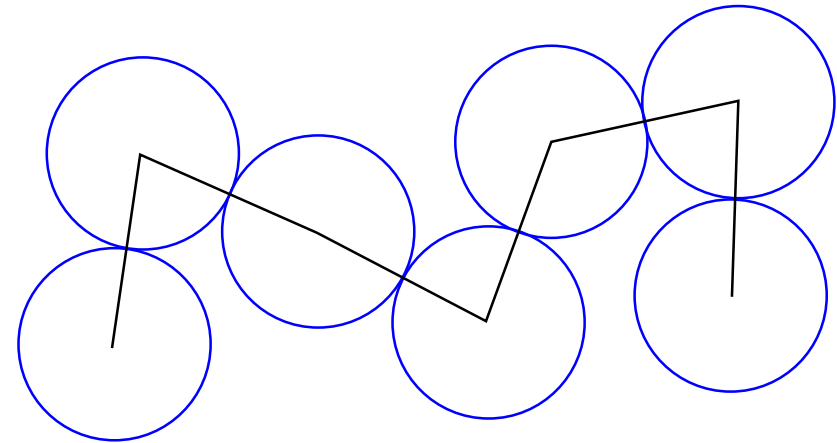
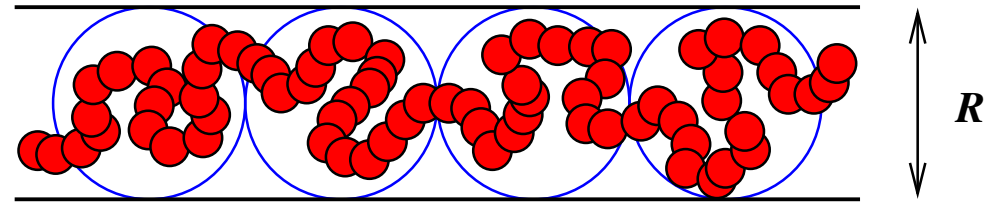
Chain /w N monomers of diam. σ



Translocation into a laterally unbounded confinement

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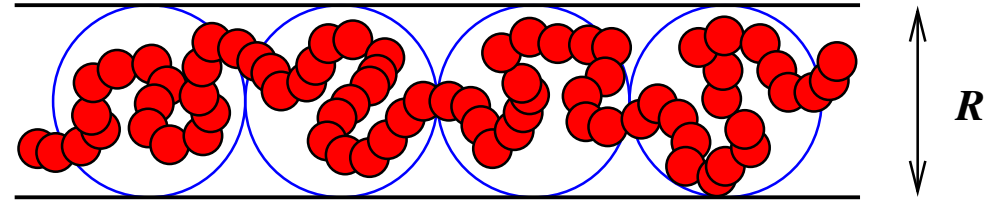
$\sigma \ll R \ll R_g$: 2D SAW of n_b blobs



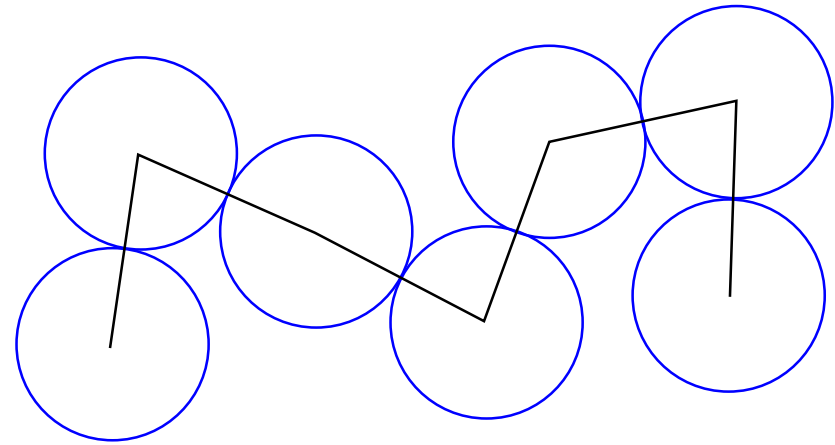
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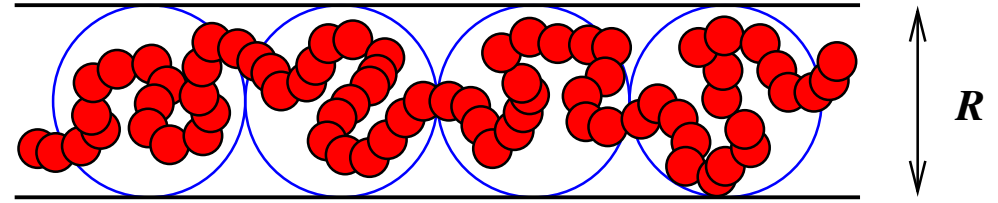
$$g = \left\{ \begin{array}{l} \text{\#monom.} \\ \text{per blob} \end{array} \right\} = \left(\frac{R}{\sigma} \right)^{1/\nu_{3D}}$$



Translocation into a laterally unbounded confinement

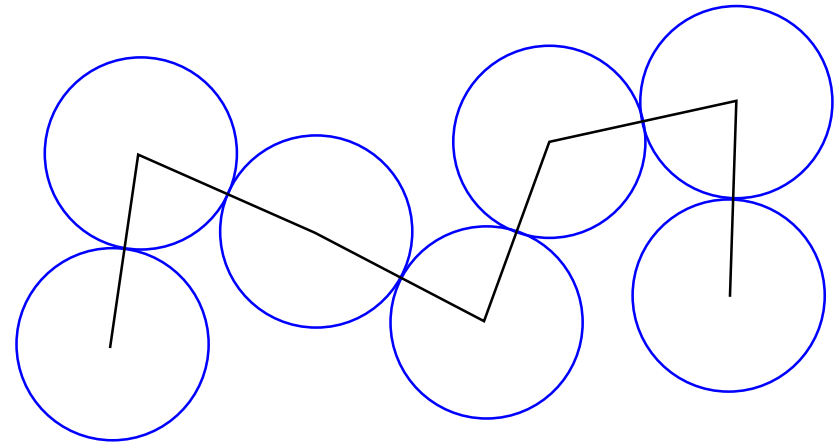
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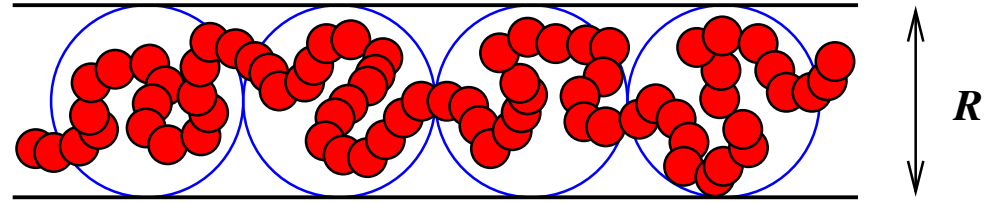
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Translocation into a laterally unbounded confinement

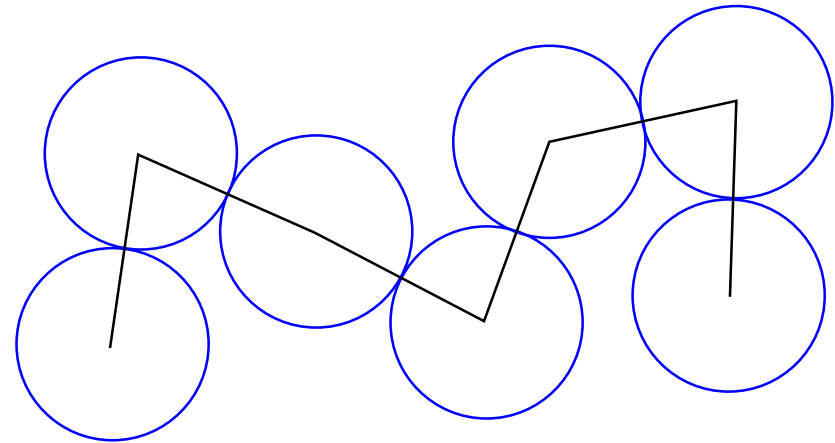
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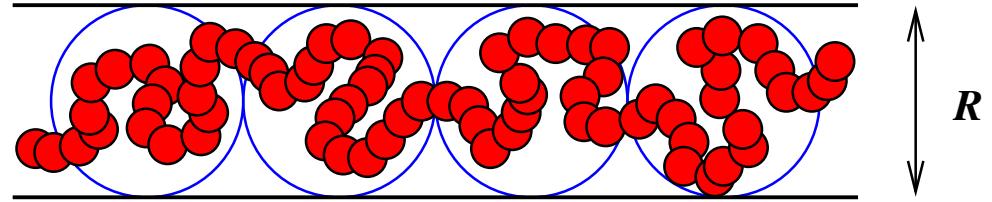
Longitudinal size of polymer:

$$R_{\parallel} \simeq n_b^{\nu_{2D}} R \simeq N^{\nu_{2D}} \sigma \left(\frac{\sigma}{R} \right)^{\nu_{2D}/\nu_{3D}-1} \simeq N^{3/4} \sigma \left(\frac{\sigma}{R} \right)^{0.28}$$

Translocation into a laterally unbounded confinement

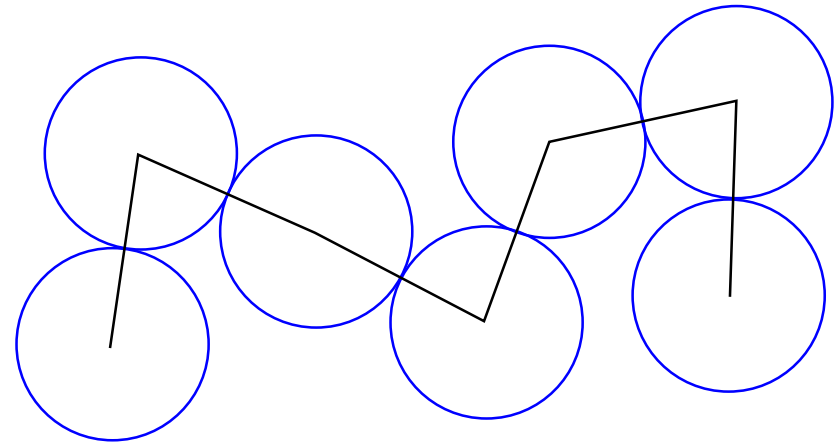
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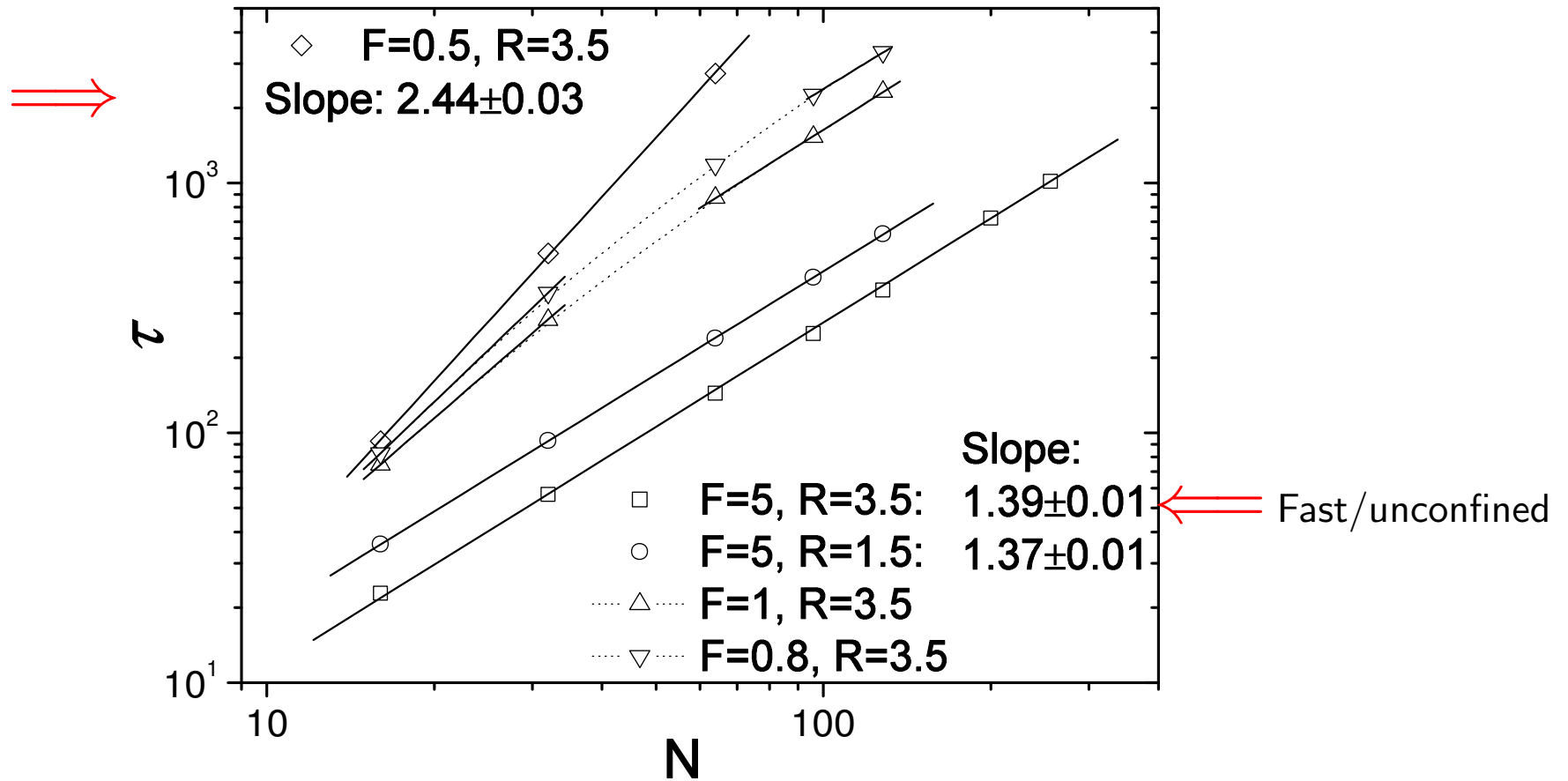
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Longit. relax. time: polymer moves by its own size (diffusivity $D \simeq 1/N$):

$$\tau_{\parallel} \simeq \frac{R_{\parallel}^2}{D} \simeq N^{1+2\nu_{2D}} R^{2(1-\nu_{2D}/\nu_{3D})} \simeq N^{2.50} R^{-0.55}$$

Translocation into a laterally unbounded confinement

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Translocation into a laterally unbounded confinement

