Dynamics of DNA in Micro/Nanofluidic Flows

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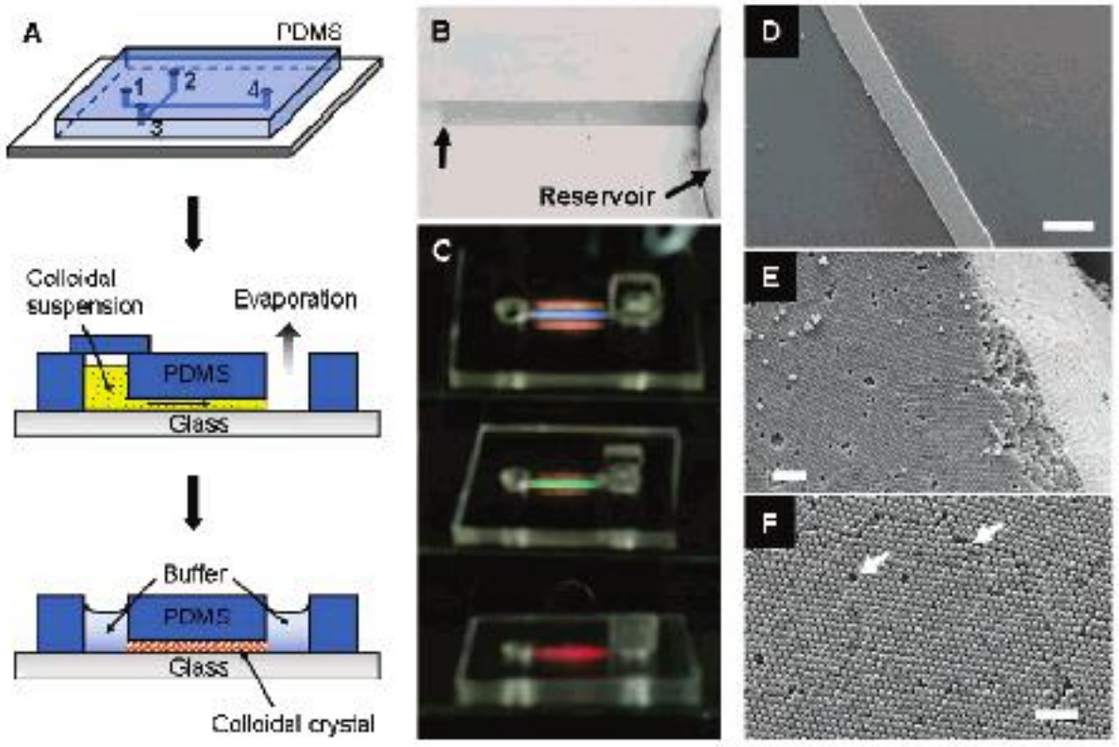
Introduction

DNA in micro/nanofluidic devices

Target systems:

- packed particles of silica



- Zeng, Harrison (2007)

- connected cavities by gel

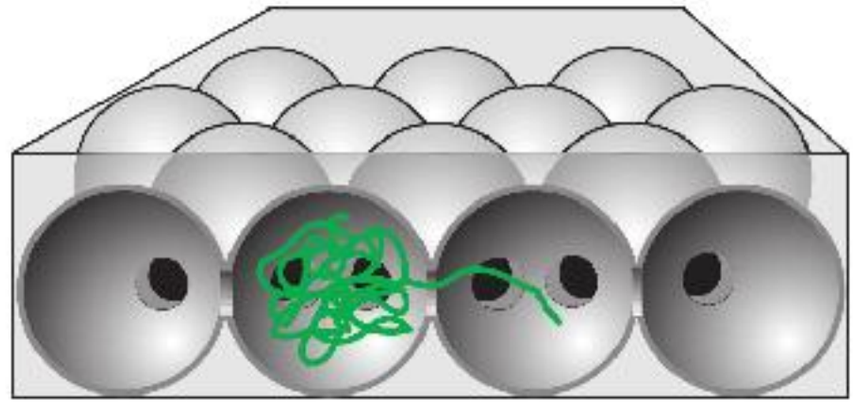


Fig. 1. Schematic of a DNA molecule trapped inside the cavity array.

- Nykypunchuk et al. (2002)
- Zeng, Harrison (2006)

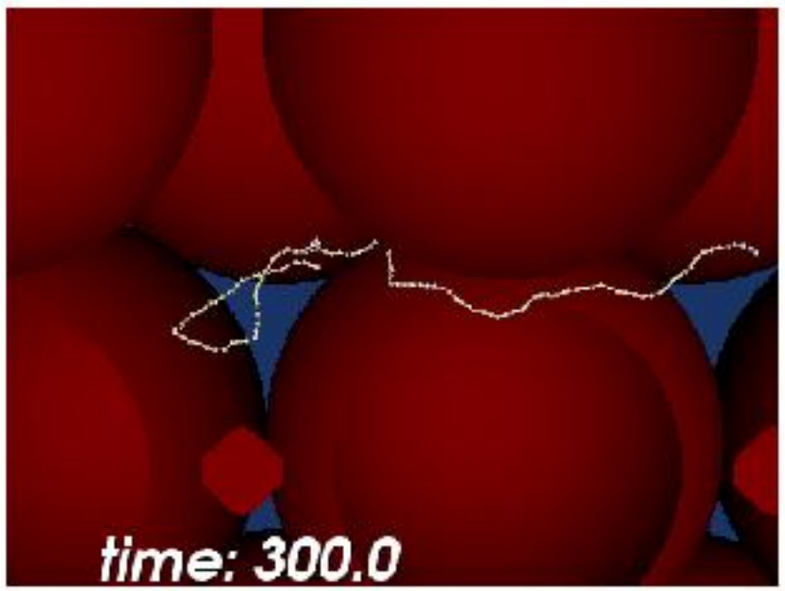
size of particle / cavity : 160nm ~ 900nm

Objective

Theory & Computation ---- Experiment

- to understand the problem,
  - what can Theor.& Comp. provide to Exp. ?
  - what do Theor.& Comp. need from Exp. ?

Theoretical Modeling



Elements:

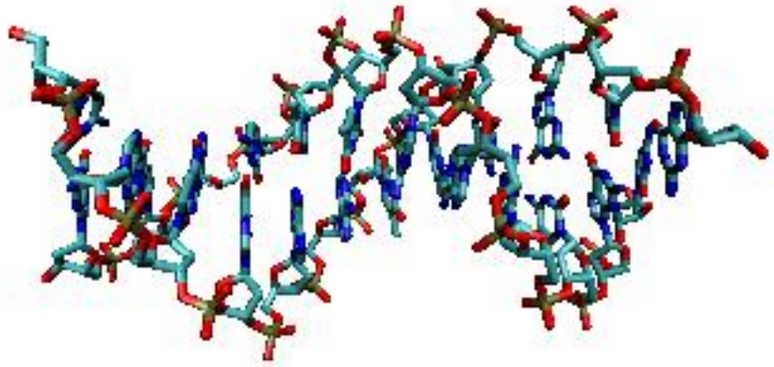
- DNA
- device (boundary)
- fluid
- electric field

Mechanisms:

- DNA model
- Brownian force
- viscous force
- electro-phoresis
- electro-osmosis
- interactions

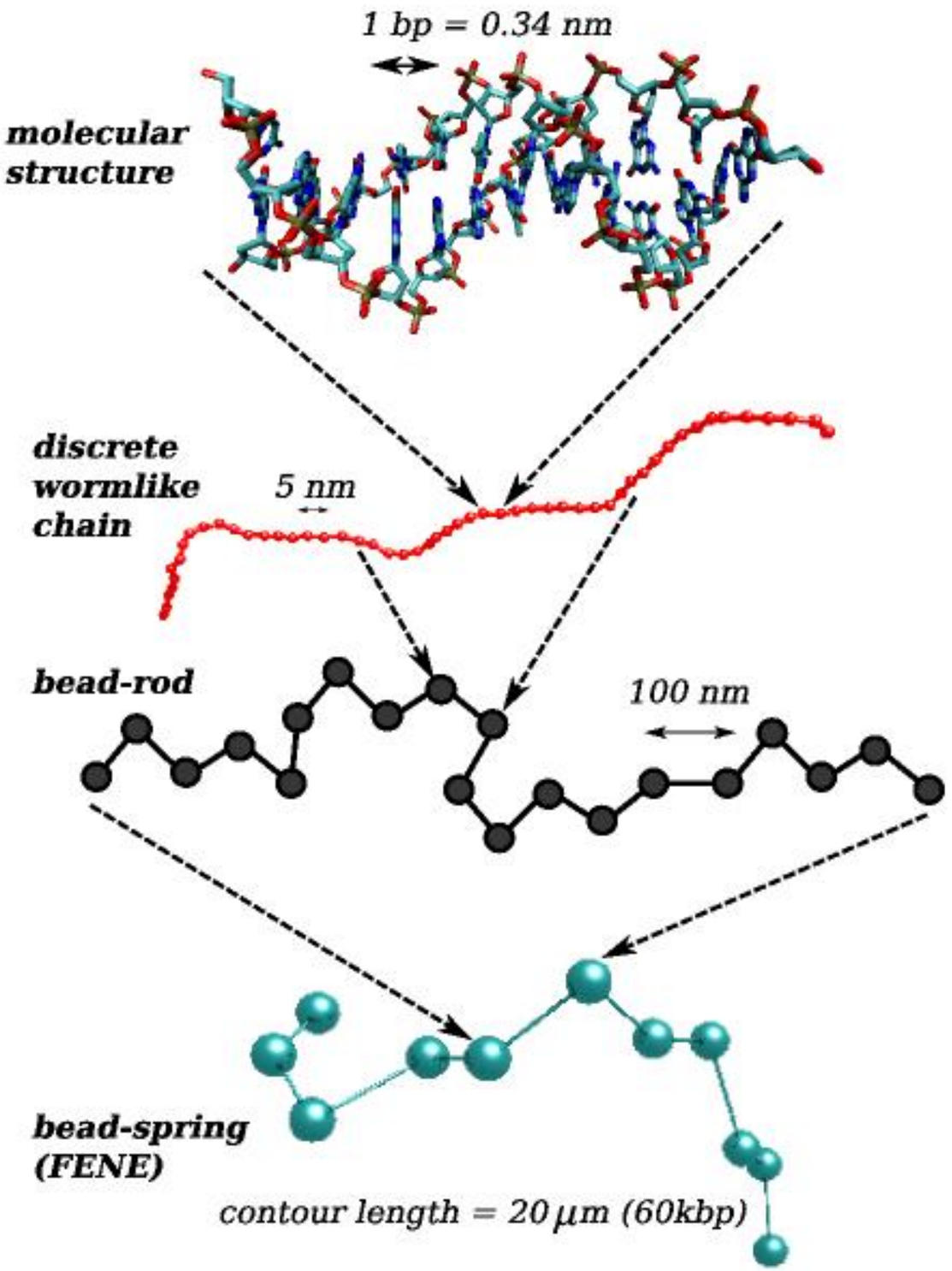
DNA

DNA for 12 bp (from 2BNA.pdb)



- size : 50bp ~ 50kbp
- contour length : 17nm ~ 17 micro m
  - (1 bp = 0.34 nm)
- DNA is not flexible
  - 1 Kuhn length = 100 nm

DNA models



molecular model

- pros : detailed
- cons : too small

dWLC model

- detailed enough
- large enough

FENE chain model

- pros : large scale
- cons : bad (confinement)

DNA models

Number of beads for dWLC and FENE models

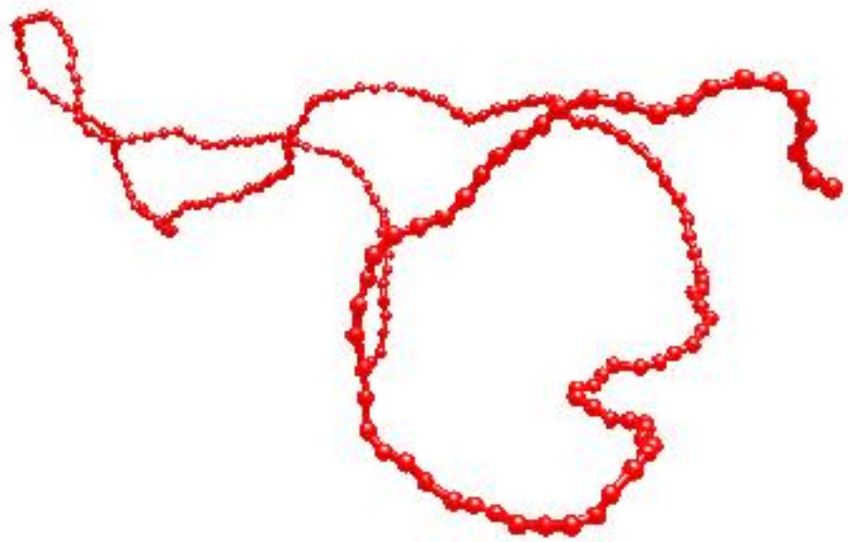
n [bp]	L [μm]	N_{dWLC}	N_{FENE}
50	0.017	3	
100	0.034	7	
200	0.068	14	
300	0.102	20	
367	0.125	25	
762	0.259	52	
1010	0.343	68	
2000	0.68	136	
2311	0.79	157	
13000	4.42	884	2
48500	16.5	3300	8
62000	21	4200	10

Brownian force

size of DNA in solution

- radius of gyration

$$R_g \propto N^{\nu}, \quad \nu \approx 0.6$$



- because of the Brownian force (thermal fluctuation)

- this is why bead-SPRING model works (entropic effect)

Brownian Dynamics

molecular dynamics (MD) vs Brownian dynamics (BD)

- Newton's equation (MD)

$$m\ddot{\boldsymbol{x}}_\alpha = \boldsymbol{F}_\alpha \qquad \Delta t^{\mathrm{MD}} = 1 \text{ fs}$$

- integrate for mom. relax. time (0.5 ps)

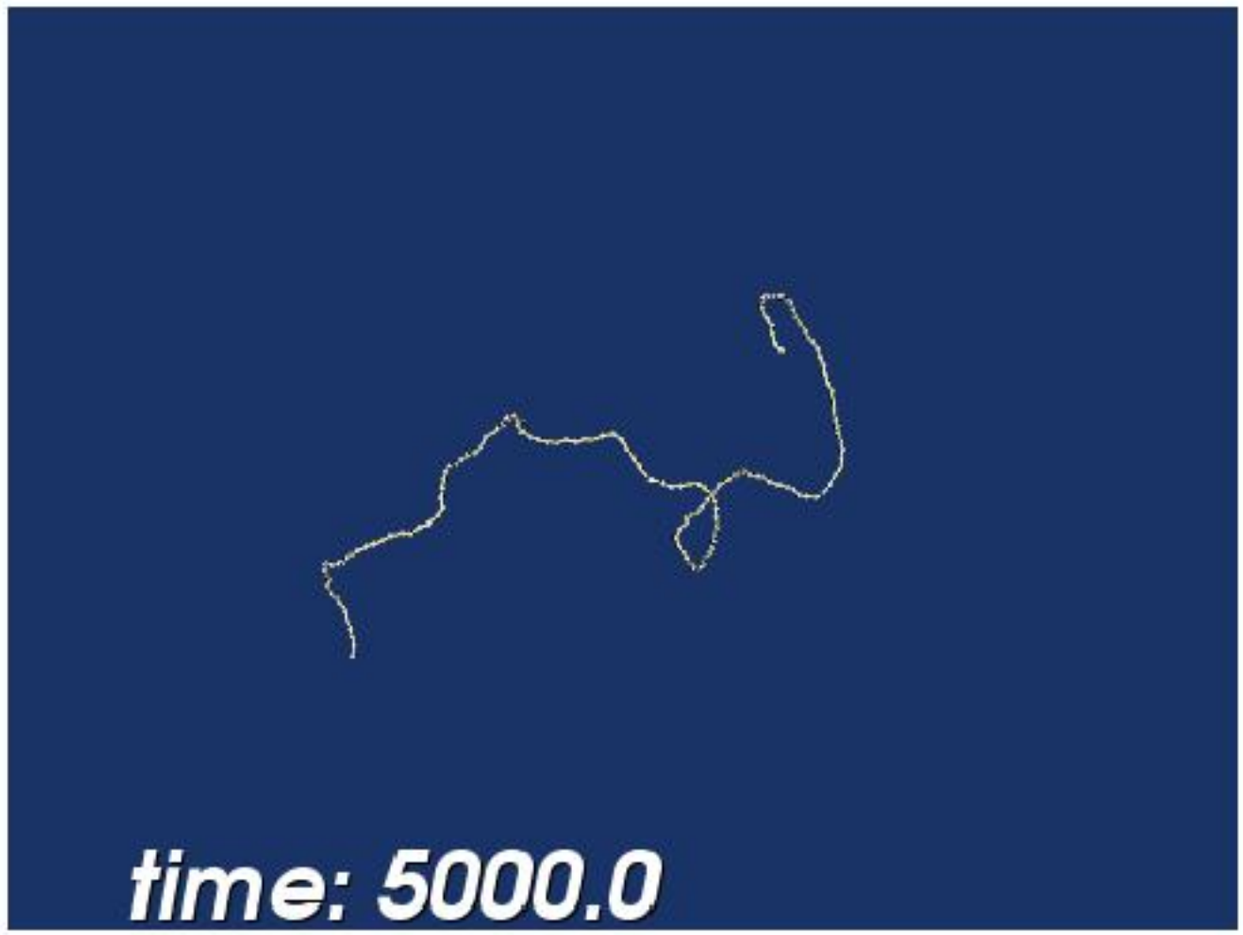
- Langevin equation (BD)

$$\Delta \boldsymbol{x}_\alpha = \boldsymbol{R}^{-1} \cdot \left(\boldsymbol{F}_\alpha + \boldsymbol{F}_\alpha^{\mathrm{B}}\right) \Delta t \qquad \Delta t^{\mathrm{BD}} = 1 \text{ ns}$$

Simulation, Part I

DNA at equilibrium

- neutral system (no electric field)



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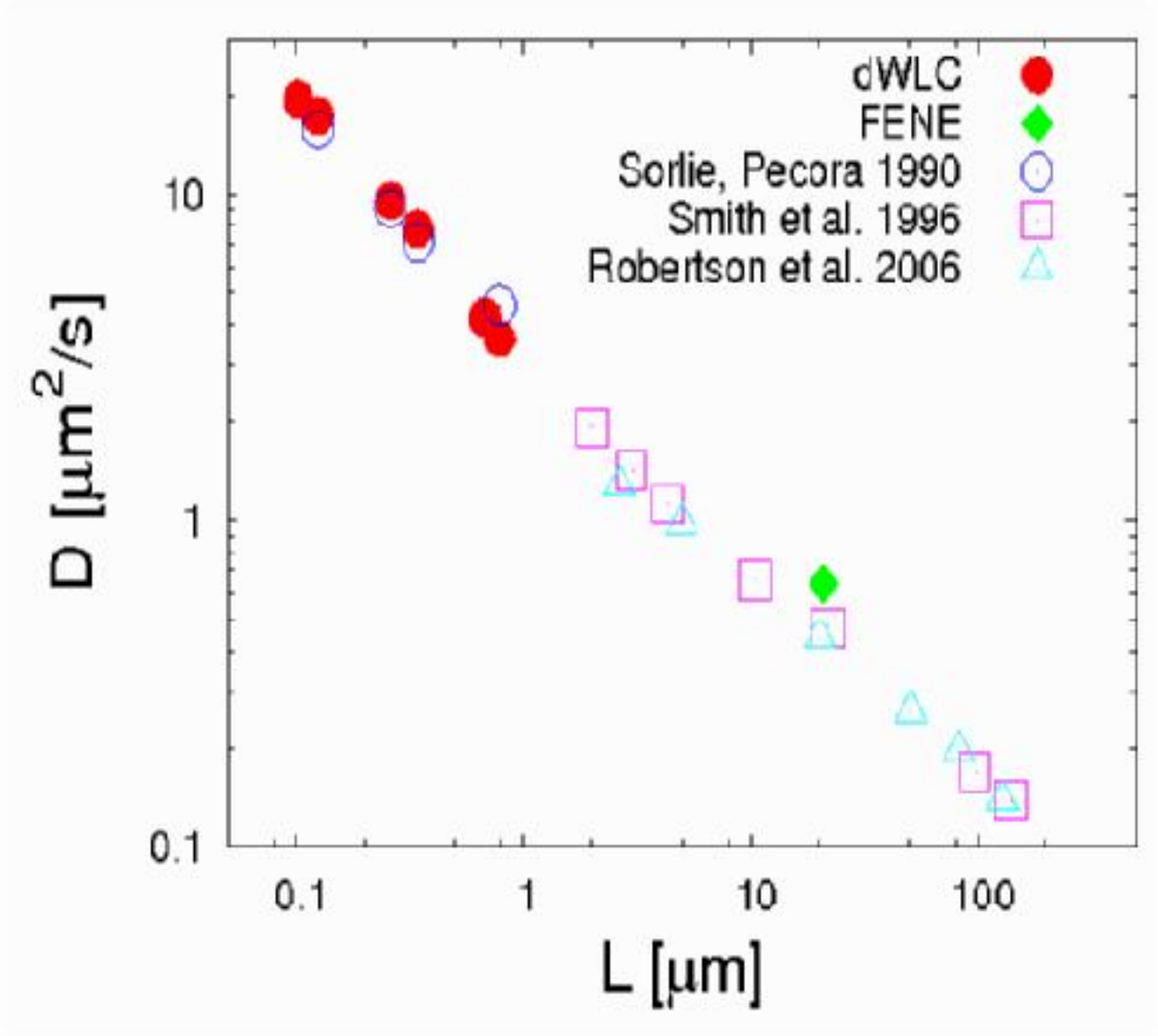
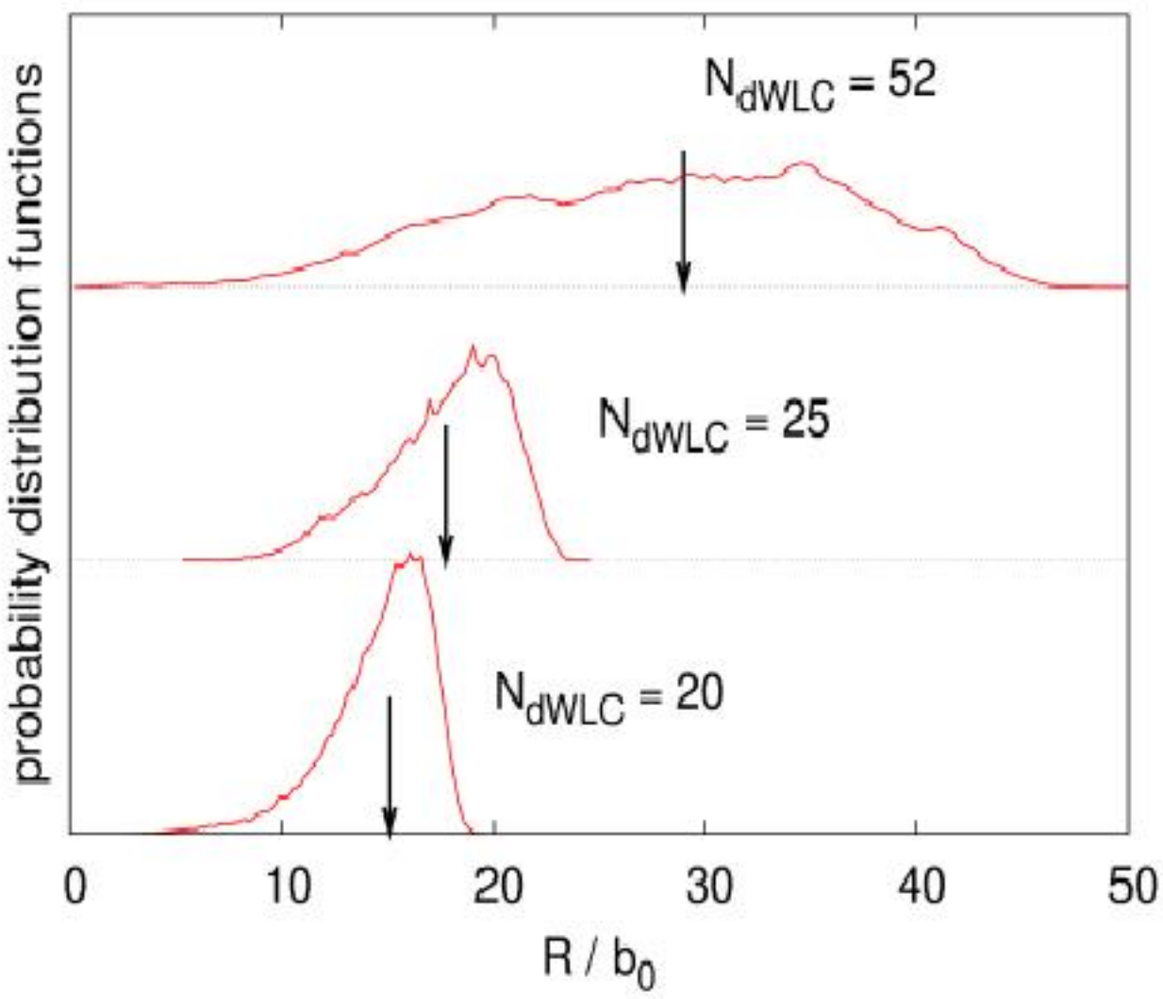
Results, Part I

What can be obtained by the simulation?

- diffusion constant



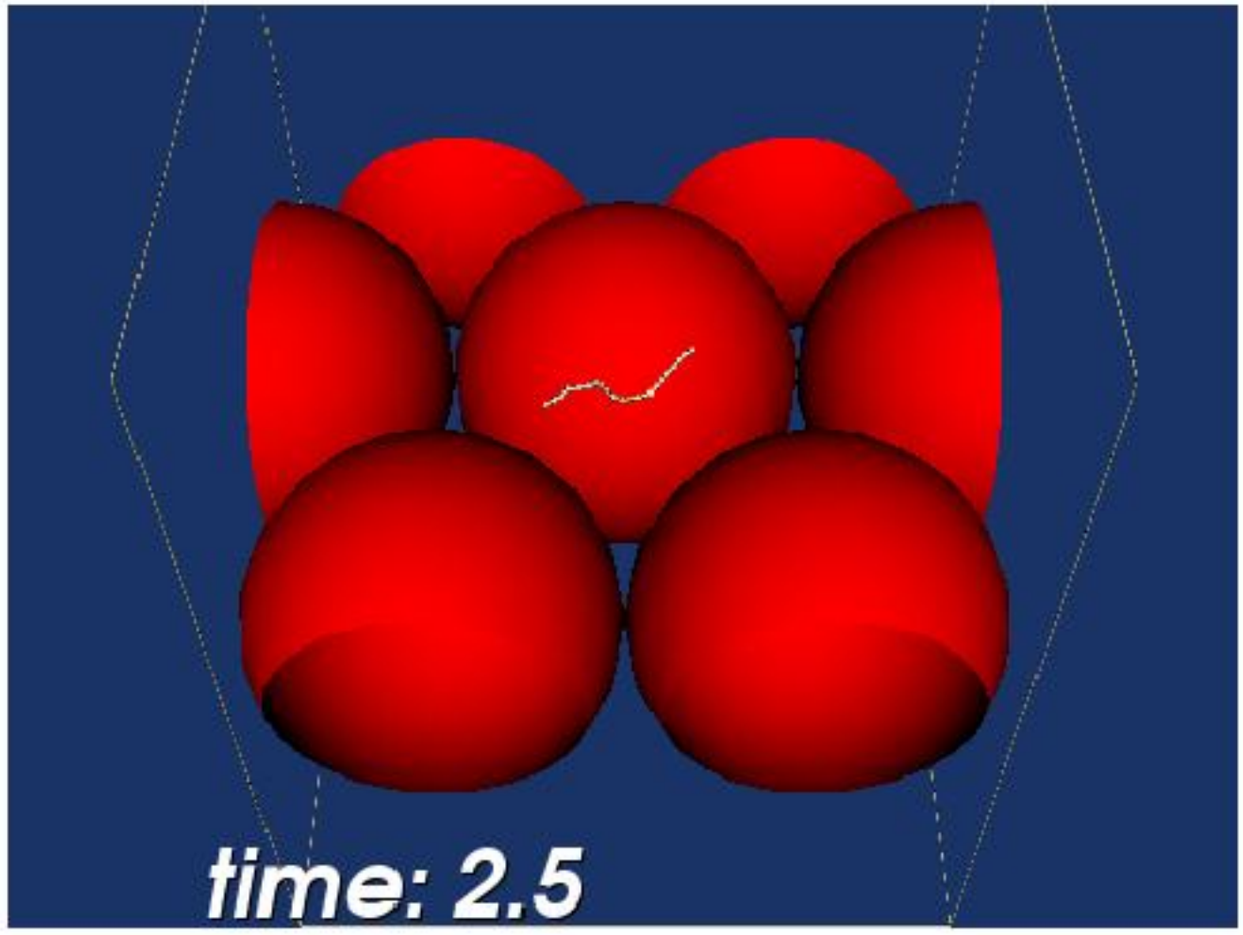
- end-to-end distance



Simulation, Part II

DNA in packed particles

- neutral system
- hydrodynamic interaction is included



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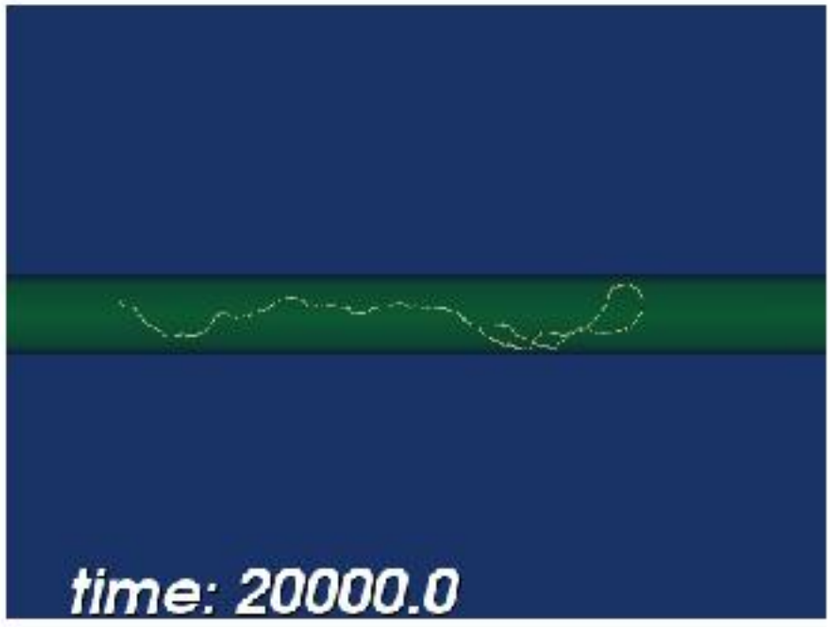
Simulation, Part III

DNA under confinement

- no HI
- spherical cavity

- cylindrical channel



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Results, Part III

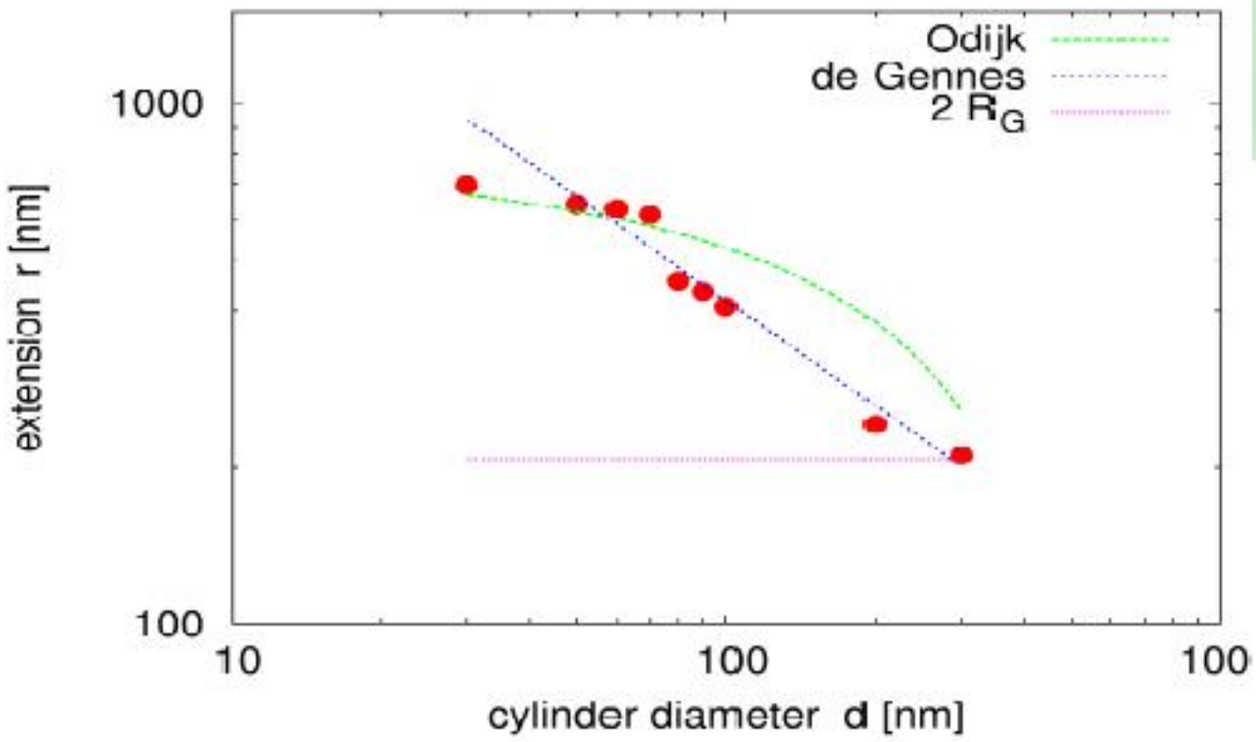
Extension under confinement

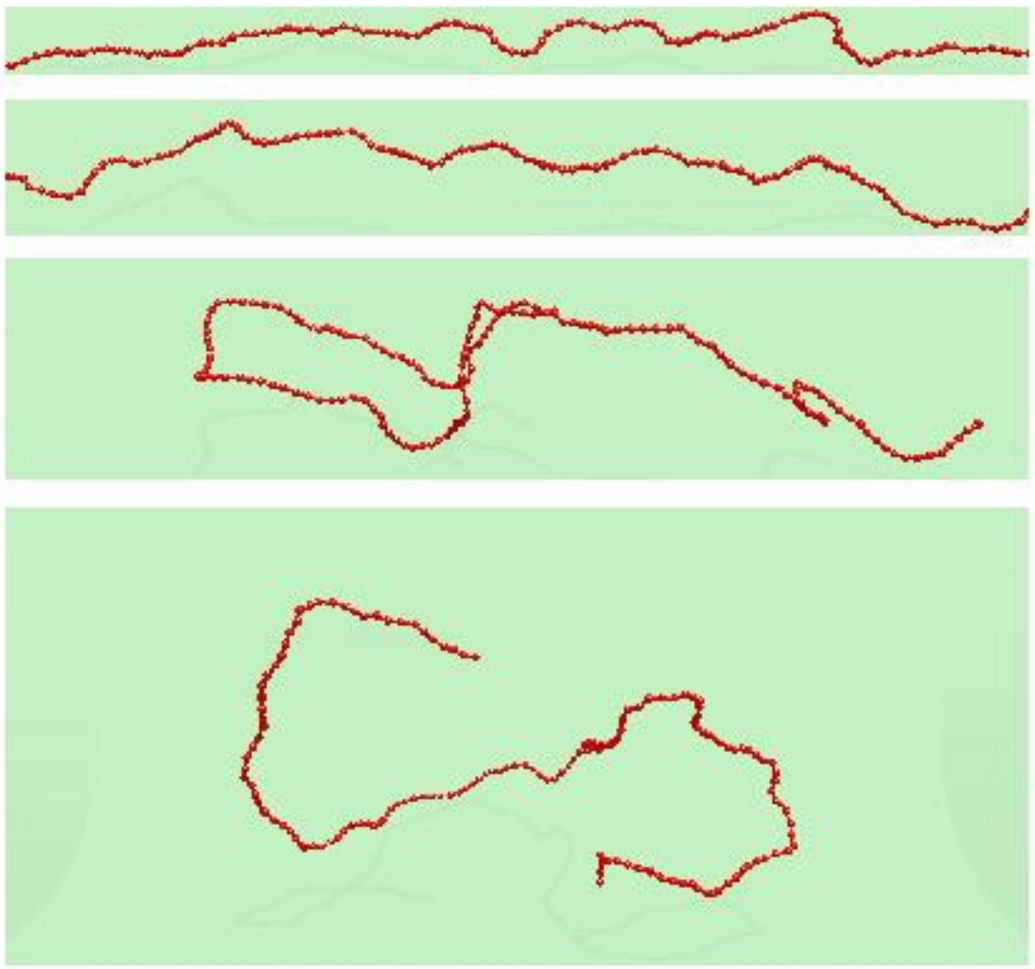
- de Gennes regime (D > P):

$$r = L\left(\frac{wP}{D^2}\right)$$

- Odijk regime (D < P):

$$r = L\left[1 - A\left(\frac{D}{P}\right)^{2/3}\right]$$





Discussions

Electric field

- Electro-phoresis and Electro-osmosis

  mobility has NO size dependence!

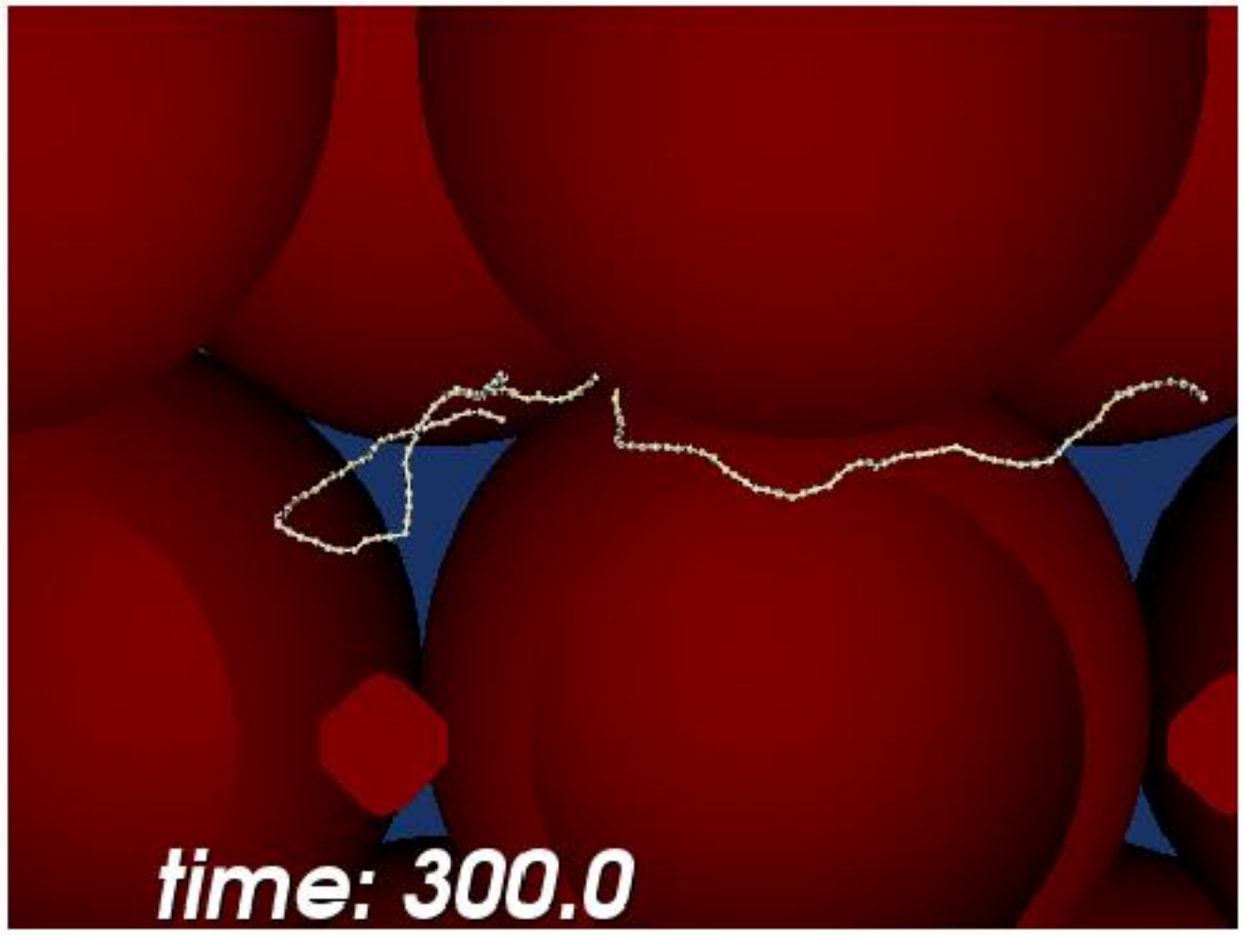
- simple model / approximation
  - EP : external force (without HI)
  - EO : imposed flow

- Experimental inputs are necessary.

Simulation, Part IV

DNA in packed particles driven by "electric field"

- EP by external force



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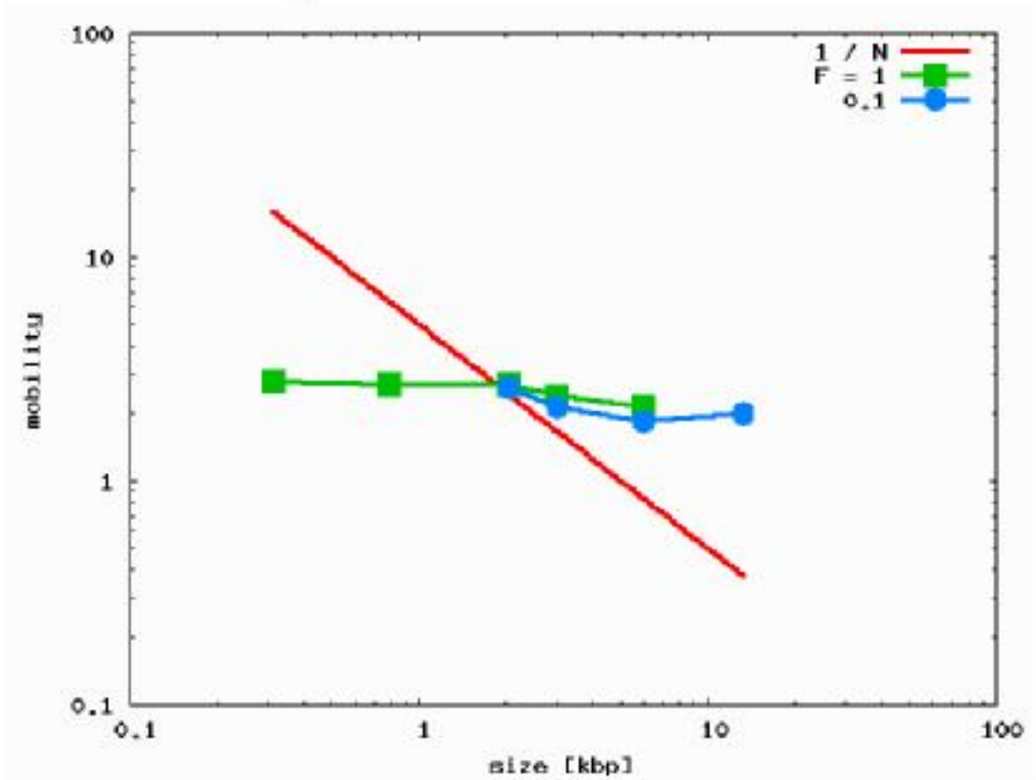
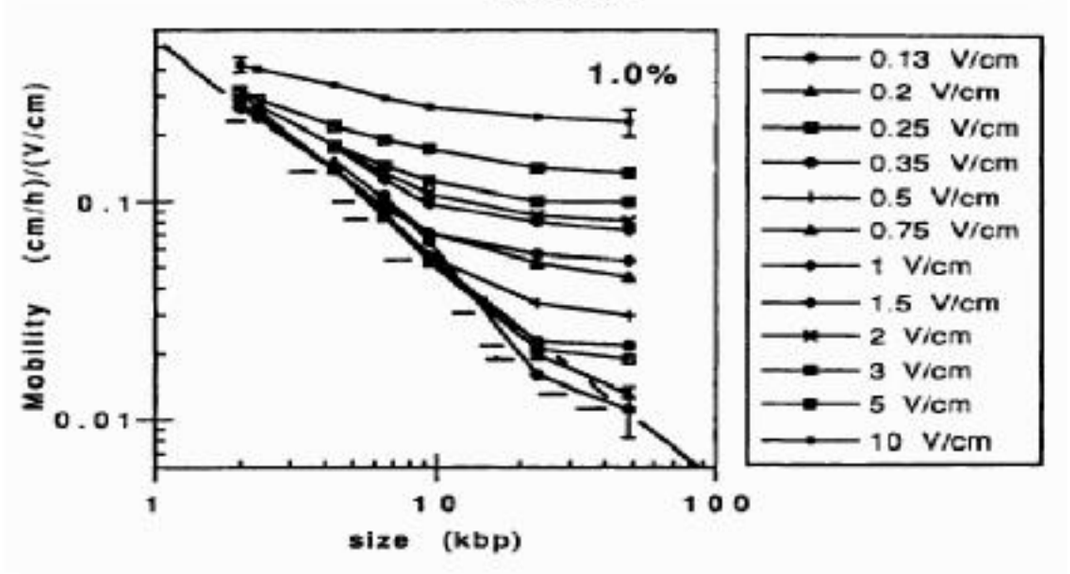
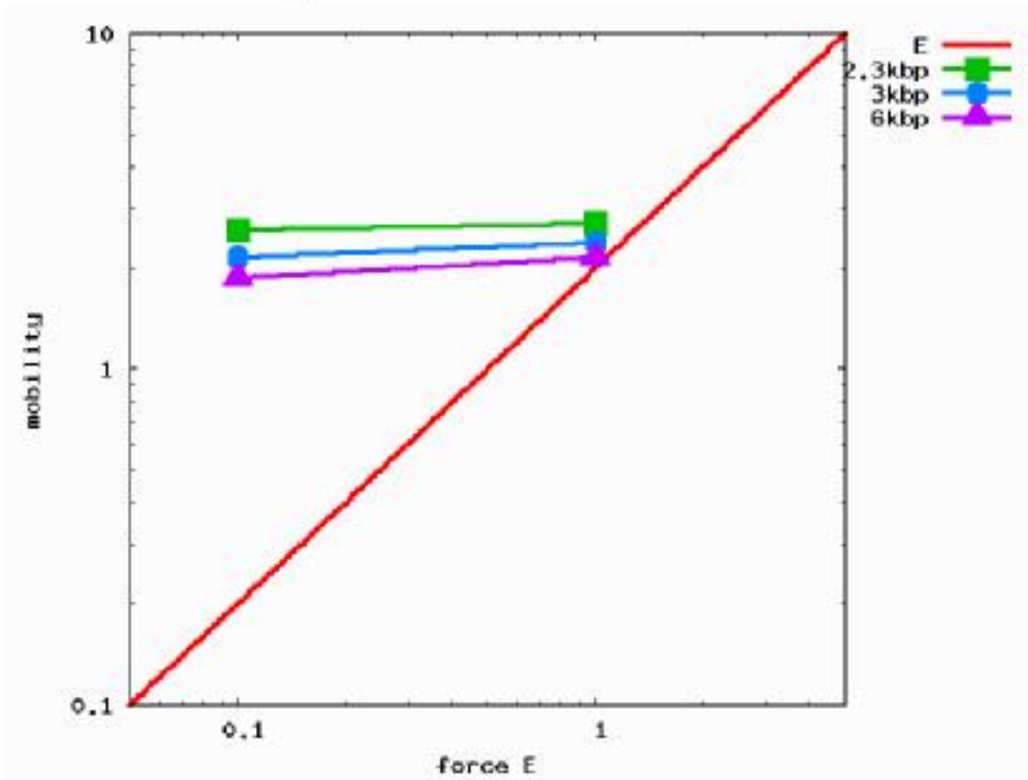
Results, Part IV

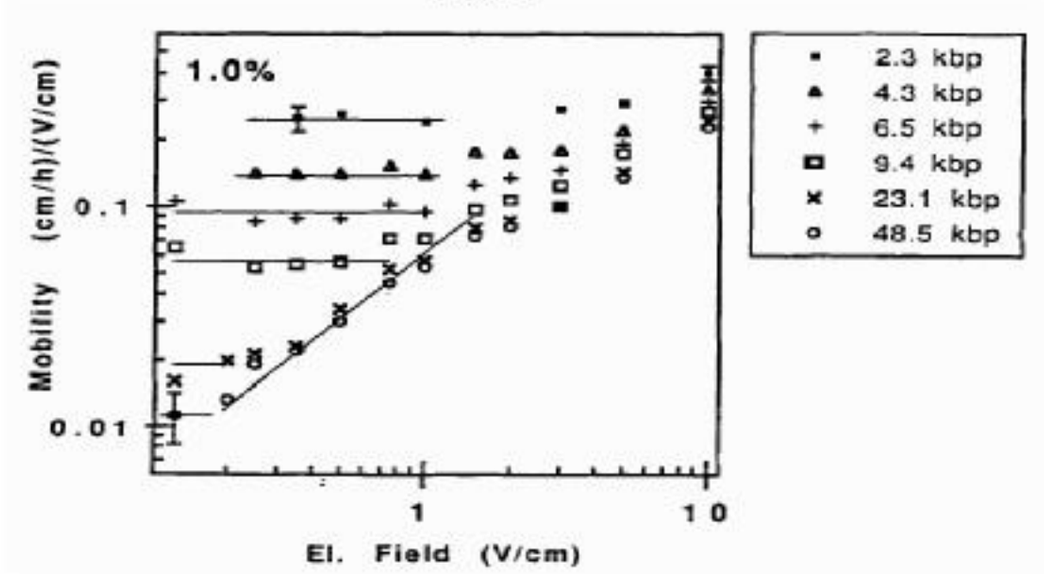
mobility vs DNA size





mobility vs force





- Heller et al. (1994)

Summary

- Brownian dynamics with dWLC model
  - OK for long DNA (not by MD)
  - good under confinement (not by bead-spring model)

- reproduce the existing results
  - diffusion constant at equilibrium
  - radius of gyration (end-to-end distance)
  - extension in confinement

- simple EP/EO model
  - size dependence on mobility

Outlook

- What Theor.& Comp. can provide ?

quantitative predictions

  - diffusion constant, radius of gyration
  - electro-phoretic mobility (passage time)
  - detailed dynamics

- Especially,

DNA-size dependence
field strength dependence
field orientation dependence