Dynamics of DNA in Micro/Nanofluidic Flows

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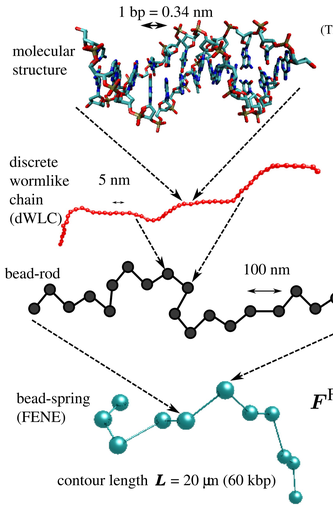
Introduction

To understand dynamics of DNAs in micro/nanofluidic devices, we use the Stokesian-Brownian dynamics method with finitely extensible nonlinear elastic (FENE) and discrete wormlike chains (dWLC).

Contrast to the molecular dynamics simulations, by the coarse-grained model, we can reach the time scale of seconds and length scale of 10-100 micrometers.

Contrast to the bulk system, the confinement in micro- and nanometer scale is essential. In nanofluidic devices, finer model (dWLC) is required.

DNA models



$$U^{\mathrm{bond}} = \frac{h}{2}\sum_i (b_i - b_0)^2$$

$$U^{\mathrm{angle}} = \frac{g}{2}\sum_i \theta_i^2$$

$$U^{\mathrm{DH}} = \frac{(\nu b_0)^2}{4\pi\epsilon\epsilon_0}\sum_{\mathrm{pairs}} \frac{\exp(-\kappa r)}{r}$$

$$\boldsymbol{F}^{\mathrm{FENE}}(\boldsymbol{r}) = \frac{k_{\mathrm{B}}T}{P}\left[\frac{1}{4}\left(1-\frac{r}{L_s}\right)^{-2} - \frac{1}{4} + \frac{r}{L_s}\right]\frac{\boldsymbol{r}}{r}$$

$$U^{\mathrm{EV}} \propto \sum_{\mathrm{pairs}} \exp\left(-\frac{r^2}{r_{\mathrm{EV}}^2}\right)$$

Stokesian-Brownian Dynamics

Equation of motion:

$$m\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = \boldsymbol{F}^{\mathrm{P}} + \boldsymbol{F}^{\mathrm{sol}} = \boldsymbol{F}^{\mathrm{P}} + \boldsymbol{F}^{\mathrm{HI}} + \boldsymbol{F}^{\mathrm{B}}$$

where $\boldsymbol{F}^{\mathrm{HI}} = -\boldsymbol{R}\cdot\boldsymbol{U}$

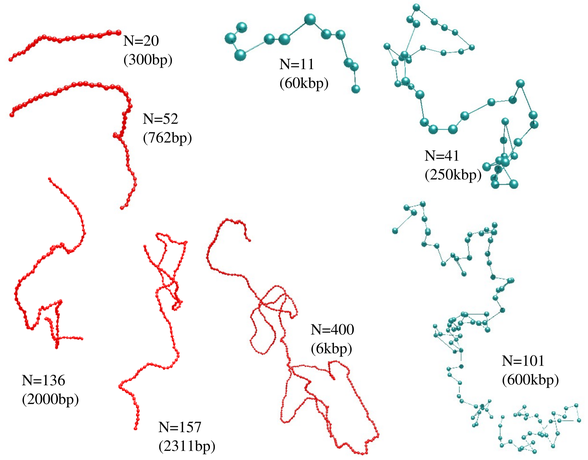
Integrating for Δt (> the momemtum relaxation time),

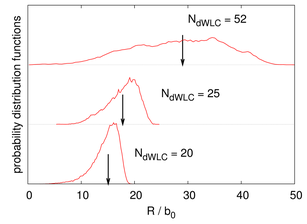
$$\Delta\boldsymbol{x} = \left[\boldsymbol{R}^{-1}\cdot\left(\boldsymbol{F}^{\mathrm{P}} + \boldsymbol{F}^{\mathrm{B}}\right) + k_B T\nabla\cdot\boldsymbol{R}^{-1}\right]\Delta t$$

$$\langle\boldsymbol{F}^{\mathrm{B}}\rangle = 0, \quad \langle\boldsymbol{F}^{\mathrm{B}}\boldsymbol{F}^{\mathrm{B}}\rangle = \frac{2k_B T}{\Delta t}\boldsymbol{R}$$

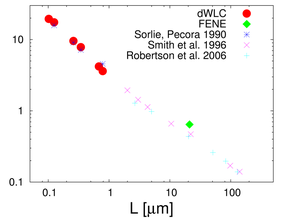
Comparing the typical time step Δt,
1 fs in MD
1 ns in SBD

DNA at Equilibrium



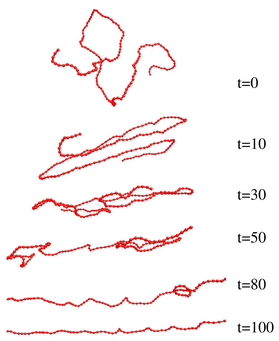


$$R^2 = \langle|\boldsymbol{x}_1 - \boldsymbol{x}_N|^2\rangle = 2LP\left[1 - \frac{P}{L}\left(1 - e^{-L/P}\right)\right]$$

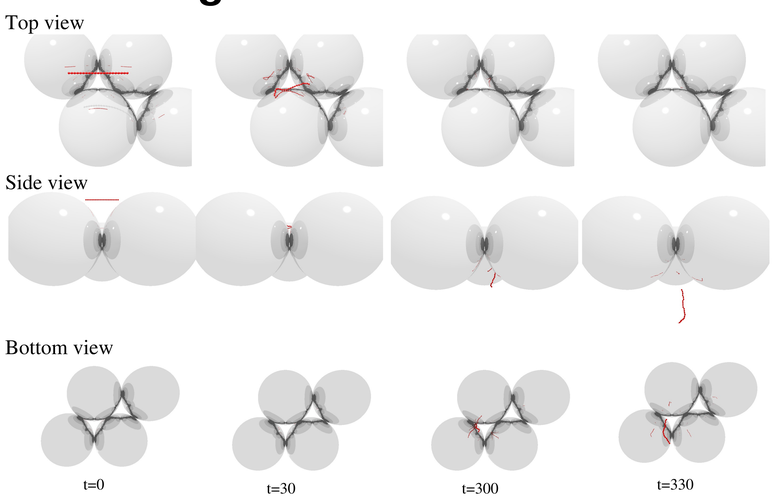


$$D = \frac{1}{6\,\Delta t}\langle|\boldsymbol{x}_{\mathrm{CM}}(\Delta t) - \boldsymbol{x}_{\mathrm{CM}}(0)|^2\rangle$$

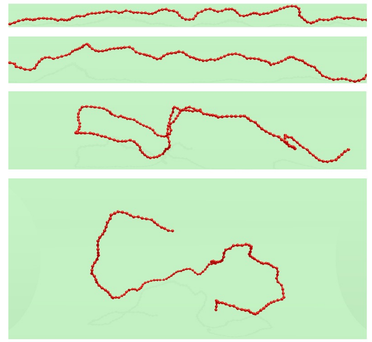
DNA in Shear Flow



DNA through Porous Matrix



DNA in Confinement

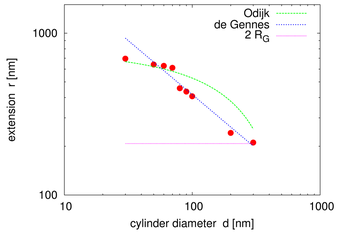


d=3, d=6 $d \ll P$ (Odijk regime) $r = L\left[1 - A\left(\frac{d}{P}\right)^{2/3}\right]$

d=10 (= P)

d=20 $d \gg P$ (de Gennes regime) $r = L\left(\frac{wP}{d^2}\right)^{1/3}$

free



Conclusions

The Stokesian-Brownian Dynamics method with FENE and dWLC models has been implemented.

The results at the equilibrium states agree well to experiments for DNAs.

The method also demonstrates for nonequilibrium states, such as in shear flow and external force.

Simple confinement (cylindrical) has been implemented.
The results agree qualitatively to the existing theories and experiments.

More complicated geometries, such as slit, porous matrix by particles, and connected cavities, will be ready shortly.

The coupling with the electric field (for electrophoresis) is in plan.

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