Nanohydrodynamics

Contents:

1. Introduction - Micro vs. Nano
2. Brownian dynamics
3. DNA model
4. Discussions (Applications)

Kengo Ichiki (UofA, NINT)

Jan 10, 2008

1. Introduction

Microhydrodynamics? Nanohydrodynamics?

Reynolds number: $Re = \dfrac{UL}{\nu}$, Peclet number: $Pe = \dfrac{6\pi\mu L^2 U}{kT}$

length	10 nm	100 nm	1 μm	10 μm
Re	10^{-8}	10^{-7}	10^{-6}	10^{-5}
Pe	10^{-3}	10^{-1}	10^{1}	10^{3}

$$\nu = \frac{\mu}{\rho} \approx 10^{-6} \quad [\mathrm{m}^2/\mathrm{s}], \quad kT \approx 4 \times 10^{-21} \quad [\mathrm{m}^2\ \mathrm{kg}\ /\ \mathrm{s}^2]$$

$$U \approx 4 \times 10^{-6} \quad [\mathrm{m}\ /\ \mathrm{s}]$$

Brownian forces

Boundary condition (no-slip => arbitrary slip)

[Lauga, Brenner, Stone (2007) in Springer Handbook of Exp. Fluid Dyn.]

1. Introduction

[Brady, Bossis (1988) Annu.Rev.Fluid Mech.]

Newton's equation of motion

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

$\boldsymbol{F}^{\mathrm{HI}} = -\boldsymbol{R}_{FU}\cdot(\boldsymbol{U}-\boldsymbol{u}^{\infty}) + \boldsymbol{R}_{FE} : \boldsymbol{E}^{\infty}$

$\boldsymbol{F}^{\mathrm{P}}$: interparticle and external forces

$\boldsymbol{F}^{\mathrm{B}}$: Brownian forces

$\langle \boldsymbol{F}^{\mathrm{B}}(0)\boldsymbol{F}^{\mathrm{B}}(t)\rangle = 2kT\boldsymbol{R}_{FU}\boldsymbol{I}$

$Pe = \infty \Rightarrow$ deterministic

$$(\boldsymbol{U} =)\,\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u}^{\infty} + \boldsymbol{R}_{FU}^{-1}\cdot\left(\boldsymbol{R}_{FE} : \boldsymbol{E}^{\infty} + \boldsymbol{F}^{\mathrm{P}}\right)$$

2. Brownian dynamics

[Ermak, McCammon (1978) J.Chem.Phys. 69, p.1352]

For $\Delta t \; > \; \tau = \dfrac{m}{6\pi\mu a}$ (relaxation time for velocity),

$$\begin{aligned} \Delta \boldsymbol{x} \;\; &= \;\; Pe \left[\boldsymbol{u}^{\infty} + \boldsymbol{R}_{FU}^{-1} \cdot \left(\boldsymbol{R}_{FE} : \boldsymbol{E}^{\infty} + \boldsymbol{F}^{\mathrm{P}} \right) \right] \Delta t \\ &\quad + \boldsymbol{\nabla} \cdot \boldsymbol{R}_{FU}^{-1} \Delta t + \boldsymbol{X}(\Delta t) \end{aligned}$$

$\langle \boldsymbol{X}\boldsymbol{X} \rangle = 2\boldsymbol{R}_{FU}^{-1}\Delta t$

$Pe = \dfrac{\dot{\gamma} a^2}{D_0} = \dfrac{6\pi\mu a^3 \dot{\gamma}}{kT}$ (Peclet number)

length, time, force are scaled by a, a^2/D_0, $6\pi\mu a^2\dot{\gamma}$.

2. How to calculate? (1)

[Grassia, Hinch, Nitsche (1995) J.Fluid Mech. 282, p.373]

Gradient term - mid-point method:

Consider the time-integration from $\boldsymbol{x}_n$ to $\boldsymbol{x}_{n+1}$ for Δt.

1. Solve velocity for the initial config. as

$$\boldsymbol{U}_n = \boldsymbol{u}_n^{\infty} + \left(\boldsymbol{R}_{FU}^{-1}\right)_n \cdot \left(\boldsymbol{F}_n^{\mathrm{E}} + \boldsymbol{F}_n^{\mathrm{P}} + \boldsymbol{F}_n^{\mathrm{B}}\right)$$

$$\boldsymbol{x}_* = \boldsymbol{x}_n + \boldsymbol{U}_n \frac{\Delta t}{2}$$

2. Solve velocity for the mid-point config. as

$$\boldsymbol{U}_* = \boldsymbol{u}_*^{\infty} + \left(\boldsymbol{R}_{FU}^{-1}\right)_* \cdot \left(\boldsymbol{F}_*^{\mathrm{E}} + \boldsymbol{F}_*^{\mathrm{P}} + \boldsymbol{F}_n^{\mathrm{B}}\right)$$

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \boldsymbol{U}_* \Delta t$$

Actually, this gives

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \boldsymbol{U}_n \Delta t + kT \boldsymbol{\nabla} \cdot \left(\boldsymbol{R}_{FU}^{-1}\right)_n \Delta t + O(\Delta t^2)$$

2. How to calculate? (2)

Random vector

$$\langle \boldsymbol{F}^{\mathrm{B}} \rangle = \mathbf{0}, \quad \langle \boldsymbol{F}^{\mathrm{B}} \boldsymbol{F}^{\mathrm{B}} \rangle = \frac{2kT}{\Delta t} \boldsymbol{R}_{FU}$$

O(3) approach:

$$\boldsymbol{R}_{FU} = \boldsymbol{\alpha} \cdot \boldsymbol{\alpha}^{\dagger} \quad \text{(Cholesky decomposition)}$$

$$\boldsymbol{\alpha} = \begin{bmatrix} \alpha_{11} & 0 & 0 & \cdots \\ \alpha_{21} & \alpha_{22} & 0 & \cdots \\ \alpha_{31} & \alpha_{32} & \alpha_{33} & \ddots \\ \vdots & \vdots & & \ddots \end{bmatrix}$$

$$\boldsymbol{F}^{\mathrm{B}} = \sqrt{\frac{2kT}{\Delta t}} \boldsymbol{\alpha} \cdot \boldsymbol{\Psi}, \quad \boldsymbol{\Psi}\text{: Gaussian random vector}$$

2. How to calculate? (2)

[Fixman (1986) Macromolecules 19, p.1204]

O(2) approach - Chebyshev approx.

$$f(x) \approx \sum_{k=0}^{N_{\mathrm{Cheb}}} a_k C_k(x) \qquad a_k : \text{coefficients defined by } f(x)$$

$$C_k(x) : \text{Chebyshev polynomials}$$

$$\begin{aligned}
b_{N-1} &= a_{N-1} \\
b_{N-2} &= 2(d_a x + d_b) b_{N-1} + a_{N-2} \\
b_{N-n} &= 2(d_a x + d_b) b_{N-n+1} - b_{N-n+2} + a_{N-n} \quad (\text{for } n = 3, \cdots, N-1) \\
b_0 &= (d_a x + d_b) b_1 - b_2 + a_0 \quad = \sum_{k=0}^{N_{\mathrm{Cheb}}} a_k C_k(x)
\end{aligned}$$

where $\quad d_a = \dfrac{2}{x_1 - x_0}, \quad d_b = -\dfrac{x_1 + x_0}{x_1 - x_0}, \quad (x_0, x_1) :$ the range of x

2. How to calculate? (2)

[Fixman (1986) Macromolecules 19, p.1204]

O(2) approach - Chebyshev approx. (continued)

applying to the random vector,

$$\begin{aligned}
\boldsymbol{b}_{N-1} &= a_{N-1}\boldsymbol{\Psi} \\
\boldsymbol{b}_{N-2} &= 2(d_a\boldsymbol{R} + d_b\boldsymbol{1}) \cdot \boldsymbol{b}_{N-1} + a_{N-2}\boldsymbol{\Psi} \\
\boldsymbol{b}_{N-n} &= 2(d_a\boldsymbol{R} + d_b\boldsymbol{1}) \cdot \boldsymbol{b}_{N-n+1} - \boldsymbol{b}_{N-n+2} + a_{N-n}\boldsymbol{\Psi} \\
\boldsymbol{b}_0 &= (d_a\boldsymbol{R} + d_b\boldsymbol{1}) \cdot \boldsymbol{b}_1 - \boldsymbol{b}_2 + a_0\boldsymbol{\Psi} \\
&\approx \boldsymbol{R}^{1/2} \cdot \boldsymbol{\Psi}
\end{aligned}$$

$$\boldsymbol{F}^{\mathrm{B}} = \sqrt{\frac{2kT}{\Delta t}}\boldsymbol{b}_0 \quad \Rightarrow \quad \langle \boldsymbol{F}^{\mathrm{B}}\boldsymbol{F}^{\mathrm{B}} \rangle = \frac{2kT}{\Delta t}\boldsymbol{R}_{FU}$$

This algorithm contains only matrix-vector product!

3. DNA model

[Larson (2005) J.Rheol. 49, p.1]

coarse graining

molecular level

bead-rod model

bead-spring level

6 LARSON

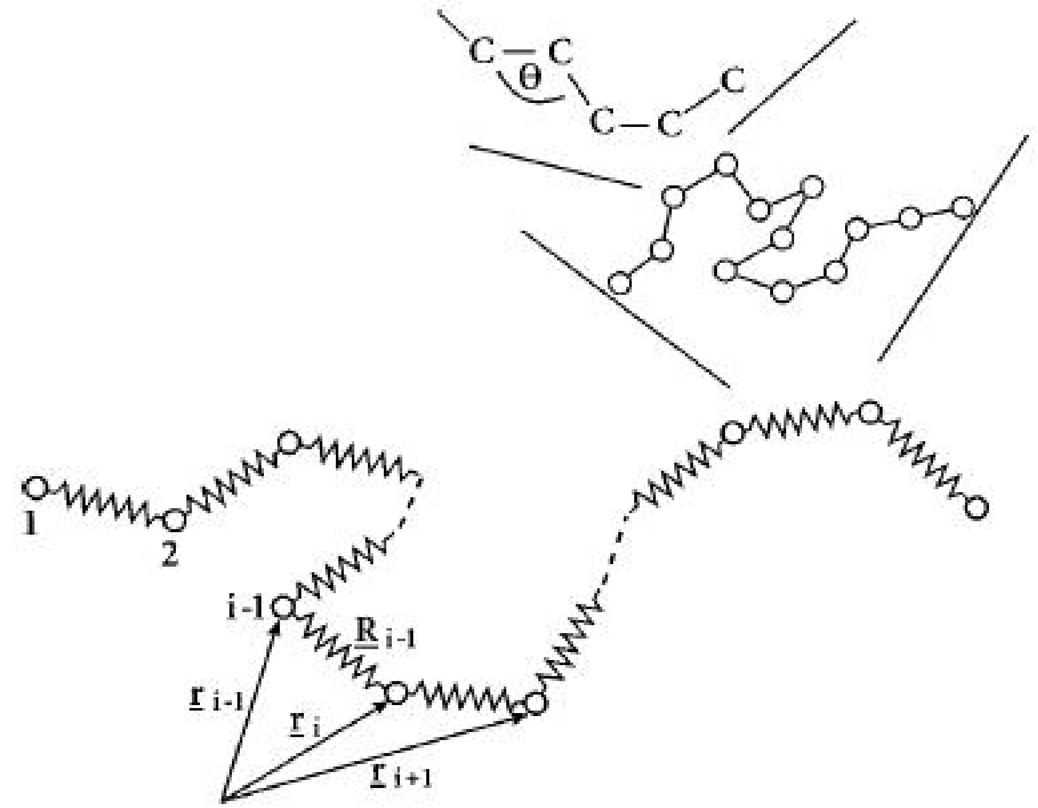
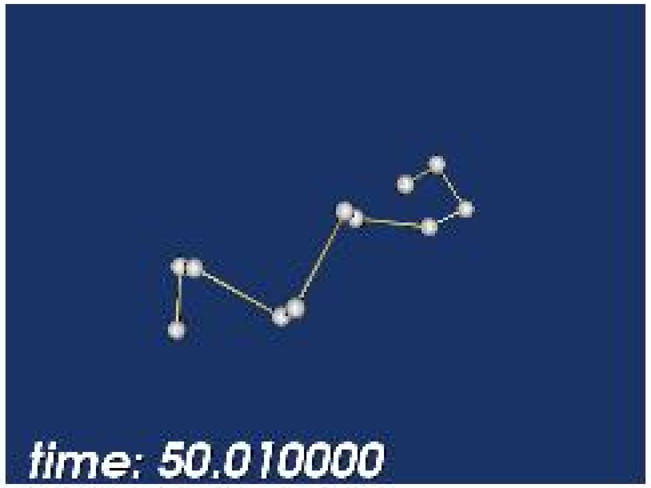


FIG. 1. Illustration of coarse-grain mapping of real polymer chain, with a carbon–carbon backbone containing fixed dihedral bond angles, onto a bead-rod chain whose configuration is that of a random walk, and further coarse-grain mapping of the bead-rod chain onto a bead-spring chain.

Other mechanisms

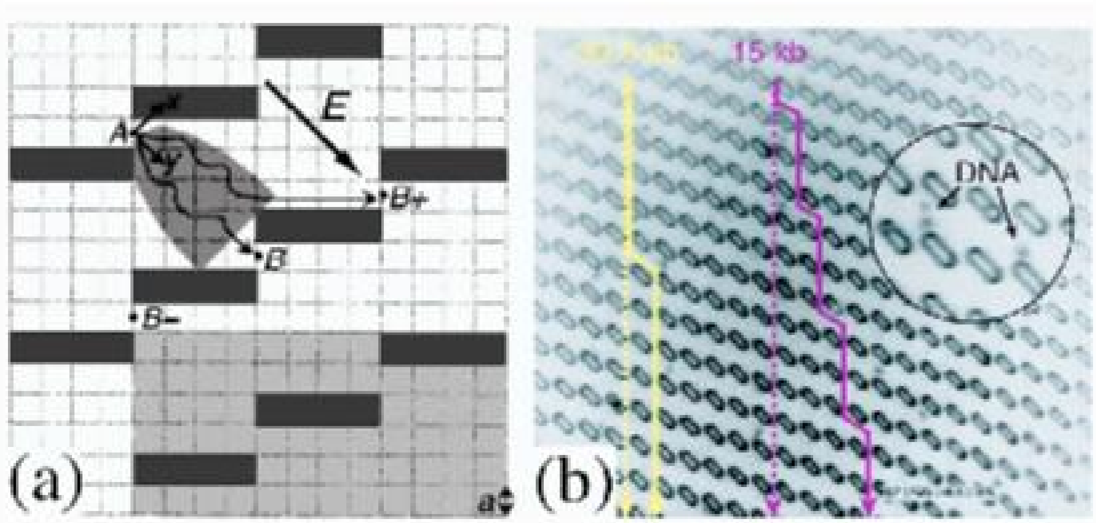
1. viscous drag
2. entropic spring
3. B - Brownian force
4. HI - hydrodynamic interaction
5. EV - excluded volume
6. IV - internal viscosity
7. SE - self-entanglement



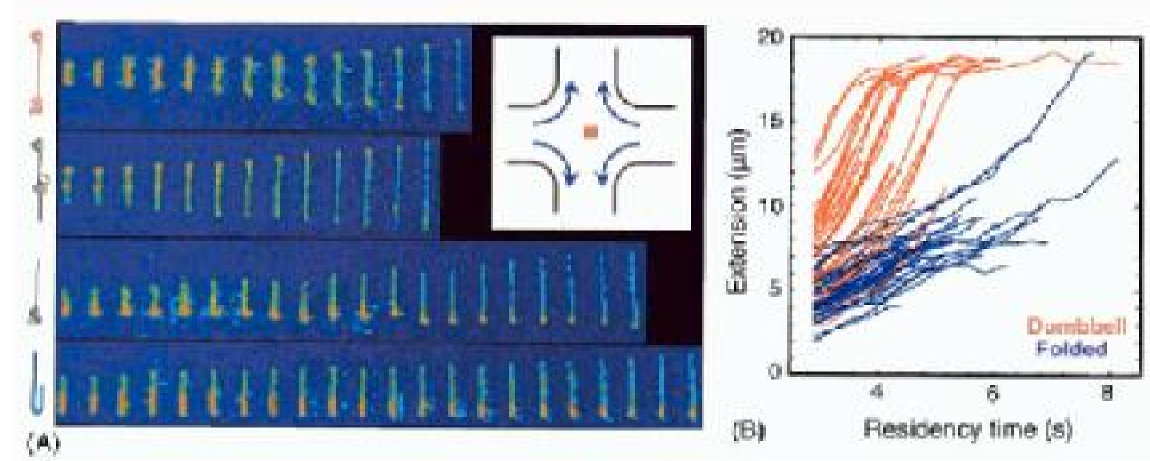
4. Discussions

Applications - Nanofluidics for DNA separations

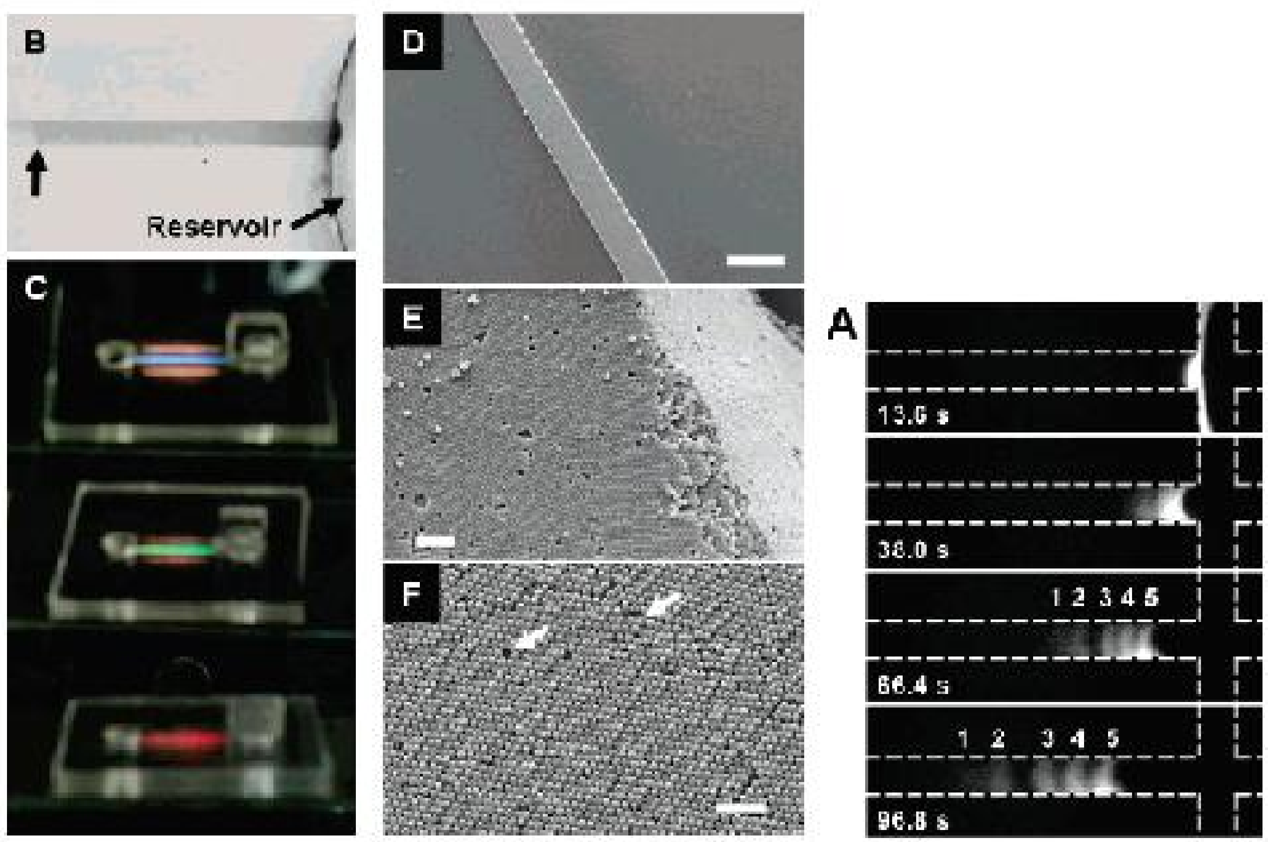
[Squires, Quake (2005) Rev.Mod.Phys.]

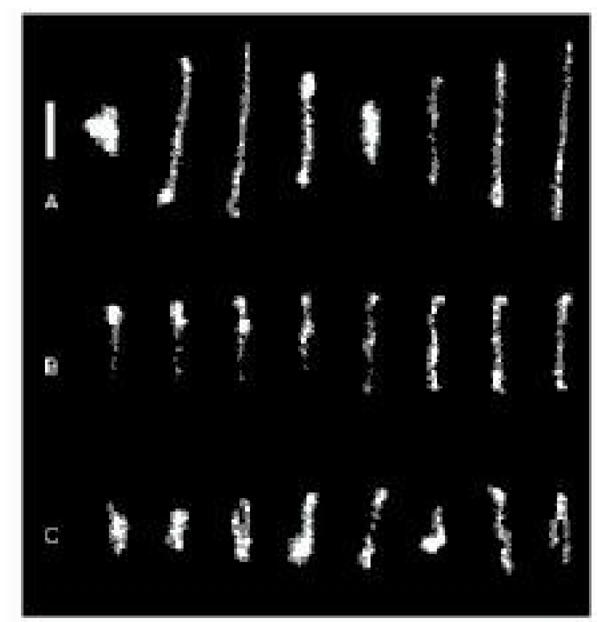


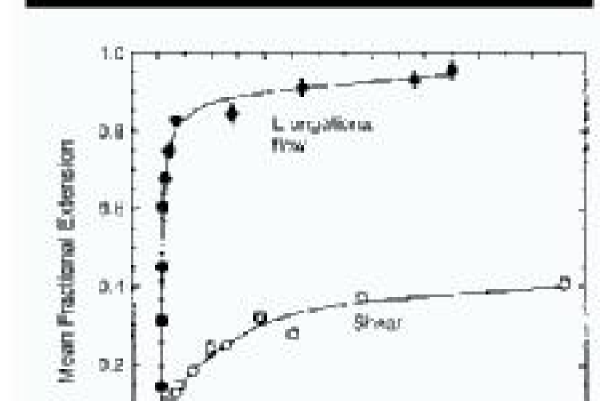
[Shaqfeh (2005) J.Non-Newtonian Fluid Mech.]



[Zeng, Harrison (2007) Anal.Chem. 79, p.2289]

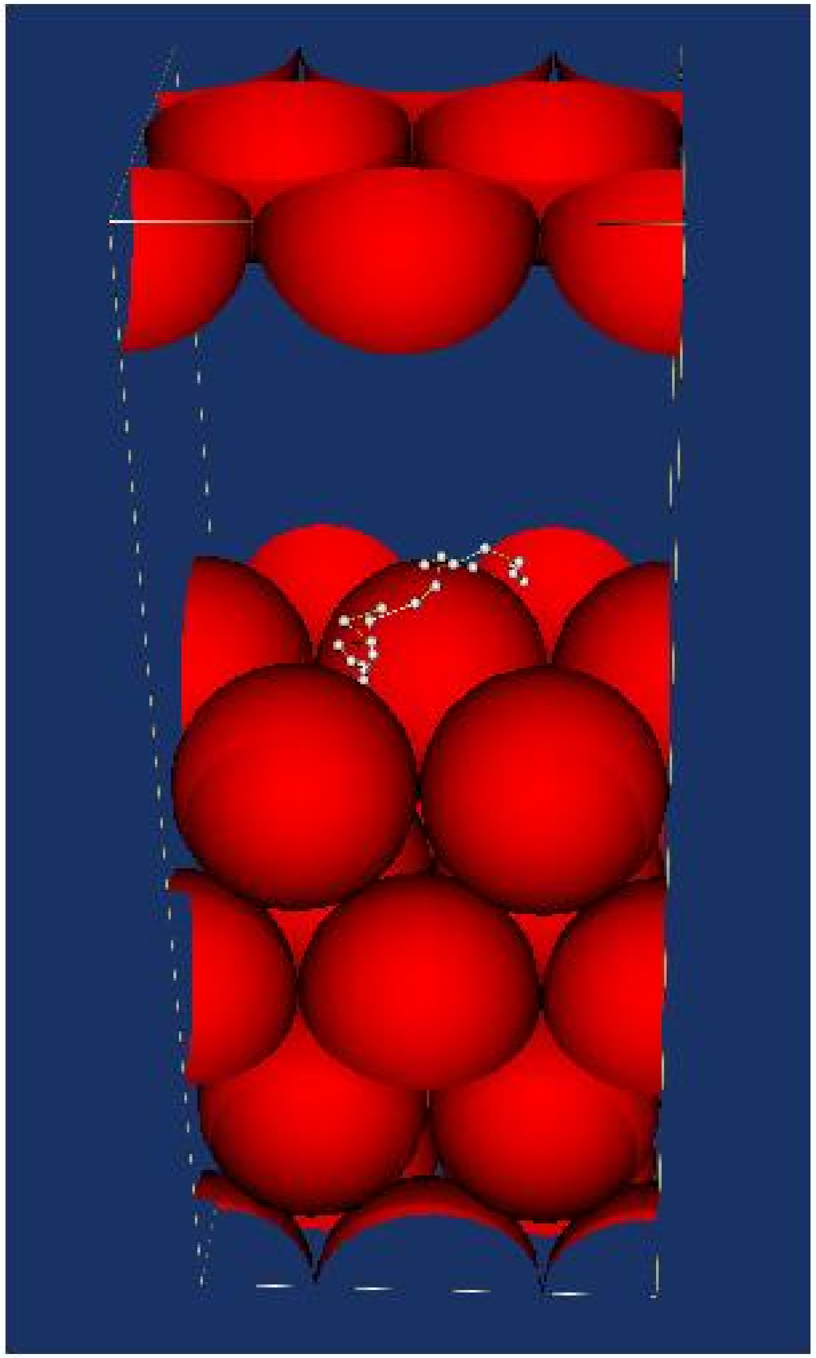






4. Discussions

Simulations



What's new?

Complicated geometry
with full HI
and Brownian force.

... TODO List

Debug, debug, debug...