Probabilistic Approach to Diffusion-mediated Surface Phenomena

Director: Denis GREBENKOV
Laboratoire PMC, Ecole Polytechnique

Yilin YE
May 15, 2023

Academic Training

- Undergraduate, Chemistry. 2015.9 - 2019.6
  Xiamen University, Xiamen, China **92.34**/100.
- Diplôme de l'ENS. 2019.9 - 2023.7
  École Normale Supérieure, Paris, France
- Research Assitant. 2020.9 - 2021.8
  Hunan University, Changsha, China
- Master 1, Chemistry. 2021.9 - 2022.7
  École Normale Supérieure, Paris, France **15.60**/20.
- Master 2, Physics, ICFP. 2022.9 - 2023.7
  École Normale Supérieure, Paris, France (1st semester) **13.70**/20,
  (2nd semester, without internship) **15.00**/20.

Course - M1

- Theoretical Chemistry: Statistical Mechanics applied to Chemistry (Damien Laage & Guilluam Stirnemann, 4 ECTS) **16.00**/20.
- Bio-Inorganic Chemistry (Clotilde Policar, 4 ECTS) **15.90**/20.
- Inorganic Materials (Gilles Wallez, 4 ECTS) **15.25**/20.
- Biophysical Chemistry of the Living Matter (Ludovic Jullien, 4 ECTS) **14.00**/20.
- Nuclear Magnetic Resonance (Kong Ooi Tan, 4 ECTS) **14.00**/20.
- Heterogenous Catalysis (Clément Guibert, 2 ECTS) **13.80**/20.

et al.

- Introduction of QFT (Adel Bilal & Guilhem Semerjian, 6 ECTS) **13.50**/20.
- Introduction of General Relativity (Marios Petropoulos, 6 ECTS) **13.40**/20.

- Research Internship M1S2 (Thomas Salez, 18 ECTS) **17.40**/20.
  Brownian Motion near the Soft Surface Feb.∼Jul. 2022
- Research Internship L3S2 (Jérémie Caillat, 6 ECTS) **15.00**/20.
  Simulation of Vibrational ICD on Model Systems with Reduced Dimensions
  Jun.∼Jul. 2020

Courses - M2S1

- Physics of Fluids and Nonlinear Physics
  (Arnaud Antkowiak & Camille Duprat, 6 ECTS) **14.86**/20.
- Statistical Field Theory and applications
  (Adam Nahum & Xiangyu Cao, 6 ECTS) **14.44**/20.
- Computational and Data-Driven Physics
  (Alberto Rosso & Rémi Monasson, 6 ECTS) **13.70**/20.
- Soft Matter Physics
  (Anke Lindner & Vincent Démery, 6 ECTS) **13.00**/20.
- Advanced Statistical Physics for soft matter
  (Christophe Texier & Jean-Noël Aqua, 6 ECTS) **12.50**/20.

Courses - M2S2

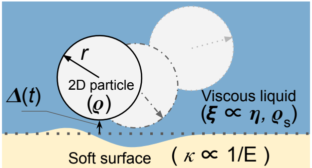
- Machine Learning (Marc Lelarge, 3 ECTS) **16.00**/20.
- Advanced Topics in Markov-chain Monte Carlo
  (Werner Krauth, 3 ECTS) **15.00**/20.
- Statistical Physics 2: Disordered Systems and Interdisciplinary Applications
  (Francesco Zamponi & Gregory Schehr, 3 ECTS) **15.00**/20.
- Conformal Field Theory
  (Benoît Estienne & Yacine IKHLEF, 3 ECTS) **14.00**/20.

- Research Internship M2S2 (Denis Grebenkov, 18 ECTS)
  Probabilistic Approach to Diffusion-mediated Surface Phenomena Apr.∼Jul. 2023

Internship - M1

ElastoHydroDynamics interactions & Modified fluctuation-dissipation relation

Equations of motion (EOM) are non-linear coupled.



$$\ddot{X}_{\mathrm{G}} + \frac{2\varepsilon\xi}{3}\frac{\dot{X}_{\mathrm{G}}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{6}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{X}_{\mathrm{G}}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{\Theta}-\ddot{X}_{\mathrm{G}}}{\Delta^{5/2}}\right] = 0$$

$$\ddot{\Delta} + \xi\frac{\dot{\Delta}}{\Delta^{3/2}} + \frac{\kappa\xi}{4}\left[21\frac{\dot{\Delta}^{2}}{\Delta^{9/2}} - \frac{(\dot{\Theta}-\dot{X}_{\mathrm{G}})^{2}}{\Delta^{7/2}} - \frac{15}{2}\frac{\ddot{\Delta}}{\Delta^{7/2}}\right] = 0$$

$$\ddot{\Theta} + \frac{4\varepsilon\xi}{3}\frac{\dot{\Theta}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{3}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{X}_{\mathrm{G}}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{X}_{\mathrm{G}}-\ddot{\Theta}}{\Delta^{5/2}}\right] = 0$$

T. Salez, and L. Mahadevan, *J. Fluid Mech.* **2015**, *779*, 181-196

Add random force into EOM for modified fluctuation-dissipation relation.

$$\dot{v} + f(\Delta)\ v + \kappa\ g(\dot{v}, v, \Delta) = 0 \qquad \longrightarrow \qquad \dot{v} = -\gamma_{\mathrm{eff}}\ v + \delta F/M$$

$$v_i = v_{i0} + \kappa \cdot v_{i1} \longrightarrow \langle v_{i0} v_{i1}\rangle\,(t,\kappa)$$

$$\gamma_i = \gamma_{i0}(\Delta) + \kappa \cdot \gamma_{i1}(\Delta) \longrightarrow \text{noise correlator amplitude}$$

$$\delta F_i = \delta F_{i0} + \kappa \cdot \delta F_{i1} \longrightarrow \langle \delta F_{i0}\delta F_{i1}\rangle\,(\kappa)$$

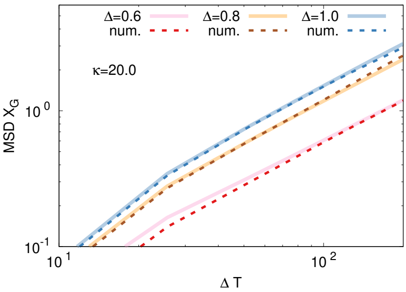
$$\boxed{\langle \delta F_i(\tau_1)\delta F_i(\tau_2)\rangle \propto 2k_{\mathrm{B}}T\ m_i\ \gamma_{i0}\ \delta(\tau_1-\tau_2)\cdot\left[1-\kappa\cdot\frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)}\right]}$$

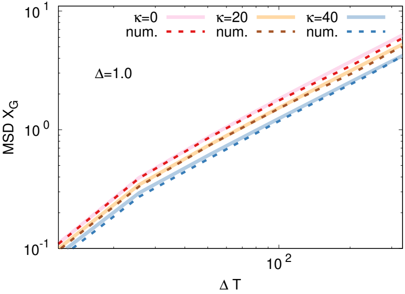
Internship - M1

Numerical simulations with **fixed** height (Δ) - Effect of compliance ($\kappa \neq 0$)

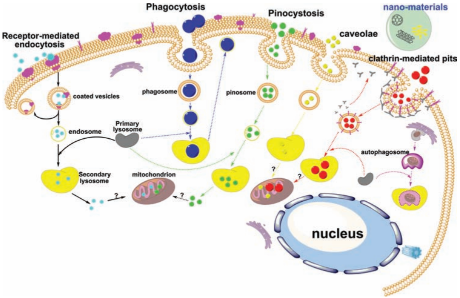
Diffusion coefficient depends on vertical positions and soft wall modulus.

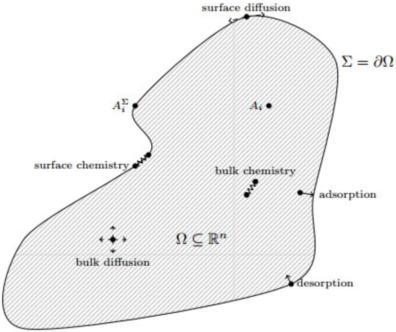
$$D(\kappa, \Delta) = D(0, \Delta)\left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)}\right]$$





Internship - M2





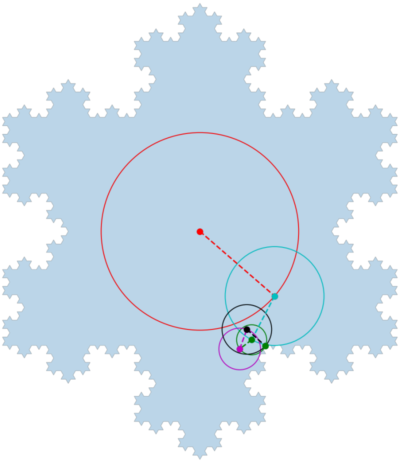
How does the complicated confining media affect the diffusion?

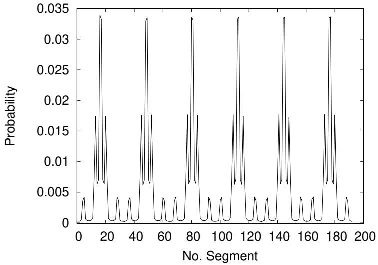
B. Augner, and D. Bothe. arXiv:1911.13030 (2019).
F. Zhao, et al. Small, 7(10), 1322-1337 (2011)

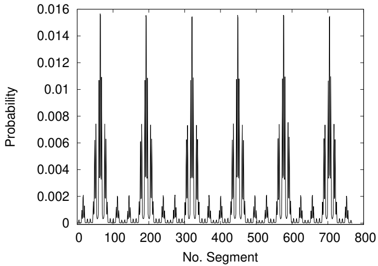
Internship - M2

Geometry-adapted fast random walk

Find minimal radius & Diffuse uniformly





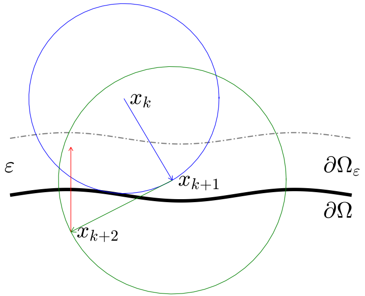


Thesis Project

$$\vec{x}_{k+1} = \vec{x}_k + \rho(\cos\theta, \sin\theta_k)$$

$$\tau = \frac{\delta^2}{4D} \qquad t_{k+1} = t_k + \tau$$

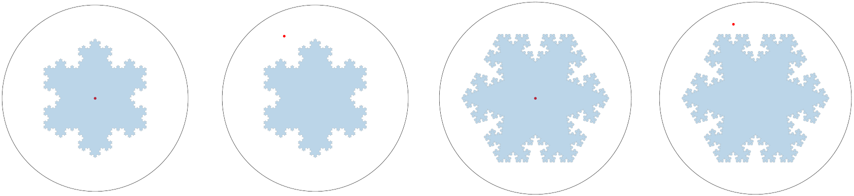
$$\ell_{t_{k+1}} = \ell_{t_k} + \sqrt{\frac{\pi}{2} D\tau}$$



- **Local Time** ℓ: How much time would one particle move near the complex surface?
- "Target-finding" diffusion near the surface;
- Collective effect of multiple independently diffusing particles;

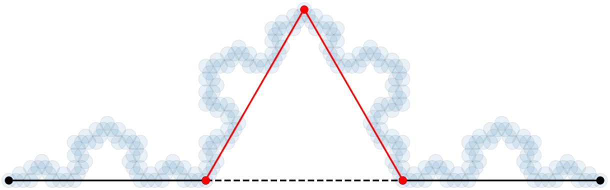
Y. Zhou, et al. Comm. Math. Sci., 15, 237-259 (2017).
Y. Lanoiselée, et al. Nature Commun. 9, 4398 (2018).

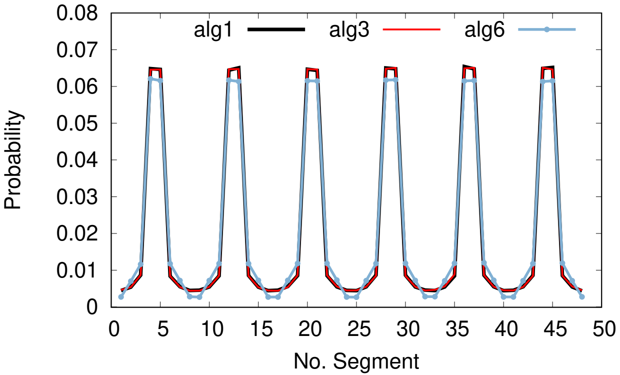
Programme



- Efficient numerical methods towards different cases;
- Diffusion on the surface & Local residence time;
- Reversible reactions controlled by diffusion on the surface;
- From 2D model to 3D model;

Thanks for your attention!




alg1
alg3
alg6
Probability
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
5
10
15
20
25
30
35
40
45
50
No. Segment