Audition ED IP Paris - Concours commun

Probabilistic Approach to Diffusion-Mediated Surface Phenomena

Director: **Denis GREBENKOV**
Laboratoire PMC, Ecole Polytechnique

Yilin YE

May 15, 2023

Academic Training

- Undergraduate, Chemistry. 2015 - 2019
  Xiamen University, Xiamen, China **92.34**/100

- Diplôme de l'ENS. (International Selection) 2019 - 2023
  École Normale Supérieure, Paris, France In progress

  - ⋆ Research Assitant. 2020 - 2021
    Hunan University, Changsha, China

  - ⋆ Master 1, Chemistry. 2021 - 2022
    École Normale Supérieure, Paris, France **15.60**/20

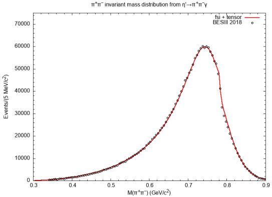
  - ⋆ Master 2, Physics, ICFP. 2022 - 2023
    École Normale Supérieure, Paris, France (1st semester) **13.69**/20
    (2nd semester, without internship) **15.00**/20

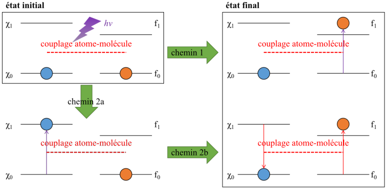
Courses Selected

- Theoretical Chemistry: **Statistical Mechanics applied to Chemistry** M1S1
  Damien Laage & Guilluam Stirnemann **16.00**/20
- **Physics of fluids and nonlinear physics** M2S1
  Arnaud Antkowiak & Camille Duprat **14.86**/20
- ⋆ **Computational and Data-Driven Physics** M2S1
  Alberto Rosso & Rémi Monasson **13.70**/20
- **Statistical Physics 2**: Disordered Systems and Interdisciplinary Applications M2S2
  Francesco Zamponi & Gregory Schehr **15.00**/20
- ⋆ **Advanced Topics in Markov-chain Monte Carlo** M2S2
  Werner Krauth **15.00**/20

Internships

- **Probabilistic Approach to Diffusion-mediated Surface Phenomena**
  M2S2, Denis Grebenkov — Apr. ∼ Jul. 2023
  Laboratoire de Physique de la Matière Condensée, Ecole Polytechnique
- **Brownian Motion near the Soft Surface** — Feb. ∼ Jul. 2022
  M1S2, Thomas Salez, Yacine Amarouchene, David Dean — **17.40**/20
  Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux
- **Study of $\eta^{(\prime)} \to \pi^+\pi^-\gamma^{(*)}$ Decays by Effective Field Theory**
  Research Assistant, Lingyun Dai — Mar. ∼ Aug. 2021
  School of Physics & Electronics, Hunan University
- **Simulation of Vibrational ICD on Model Systems with Reduced Dimensions** — Jun. ∼ Jul. 2020
  L3S2, Jérémie Caillat — **15.00**/20
  Laboratoire de Chimie Physique - Matière et Rayonnement, Sorbonne Université

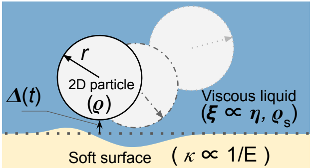




Internship - M1

ElastoHydroDynamics interactions & Modified fluctuation-dissipation relation

Equations of motion (EOM) are non-linearly coupled



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

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

$$\left\langle \delta F_i^2 \right\rangle \propto \frac{2m_i\gamma_{i0}}{\beta}\left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)}\right] \qquad \frac{D(\kappa, \Delta)}{D(0, \Delta)} = 1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)}$$

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

Internship - M1

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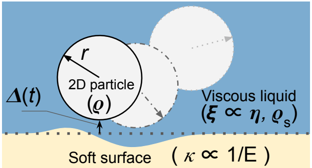

$$\ddot{X}_G + \frac{2\varepsilon\xi}{3}\frac{\dot{X}_G}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{6}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{X}_G}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{\Theta} - \ddot{X}_G}{\Delta^{5/2}}\right] = 0$$

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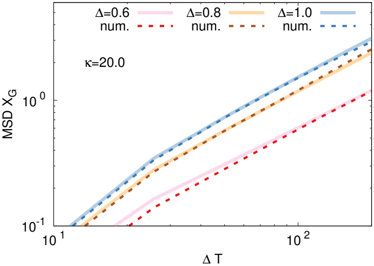
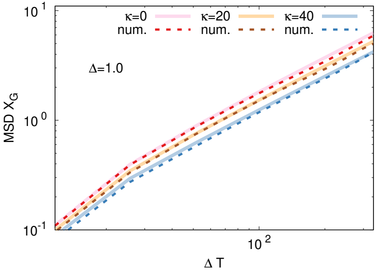
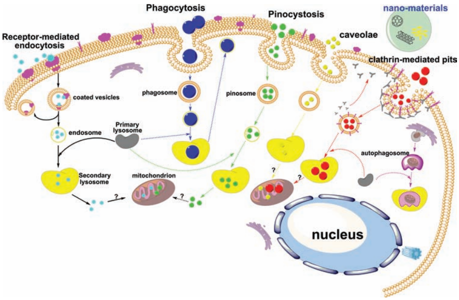
T. Salez, and L. Mahadevan, *J. Fluid Mech.* **2015**, *779*, 181-196

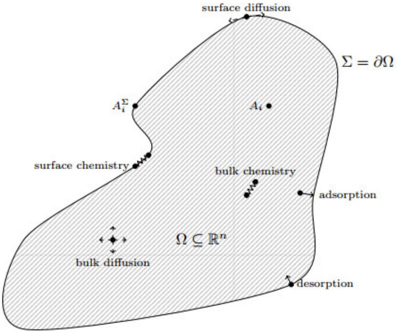
Add random force into EOM for modified fluctuation-dissipation relation





Thesis Project - Motivation





How does the complicated environment affect diffusion-controlled reactions?

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

Thesis Project

Probabilistic Approach to Diffusion-mediated Surface Phenomena

- Boundary local time ℓ_t characterizes the number of encounters with the boundary
- Surface reaction occurs when ℓ_t exceeds some threshold $\hat{\ell}$ characterized by $\Psi(\ell)$
  - ⋆ standard surface reactions $\Psi(\ell) = qe^{-q\ell}$
  - ⋆ various surface reactions: arbitrary $\Psi(\ell)$
- This approach was applied only in simple confinements like sphere.

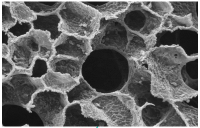
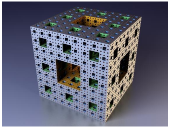
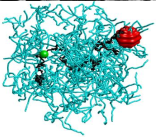
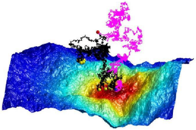
figs/pending_scheme.png

D. S. Grebenkov, Physical Review Letters 125, 078102 (2020)

Thesis Project - Aims

Probabilistic Approach to Diffusion-mediated Surface Phenomena

- Numerical practices on local time and conditional probability $P(\mathbf{x}, \ell, t|\mathbf{x}_0)$;
- Analyze reversible chemical reactions by generalized propagator $G_\Psi(\mathbf{x}, t|\mathbf{x}_0) = \int \mathrm{d}\ell \Psi(\ell) P(\mathbf{x}, \ell, t|\mathbf{x}_0)$;
- Popularize 2D model towards 3D model for simulations of real cases;

Internship - M2

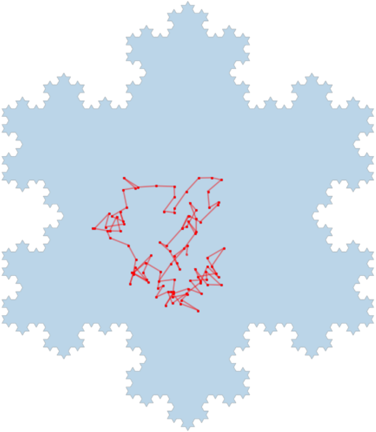
Brownian motion as Markov-chain Monte Carlo

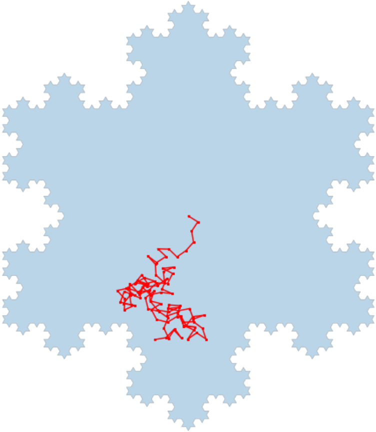
$$\delta = \text{constant}$$

$$\Delta x_i = \text{ran}(-\delta, +\delta) \qquad \Delta y_i = \text{ran}(-\delta, +\delta)$$

$$r = \text{constant} \qquad \theta_i = \text{ran}(0, 2\pi)$$

$$\Delta x = r\cos\theta_i \qquad \Delta y = r\sin\theta_i$$



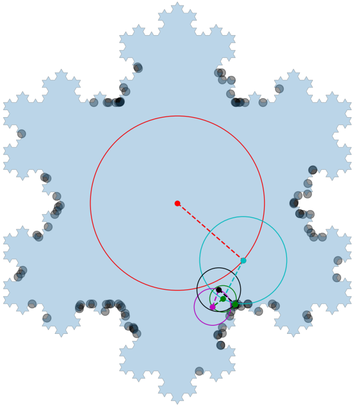


Internship - M2

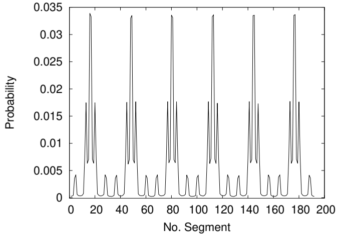
Geometry-adapted fast random walk

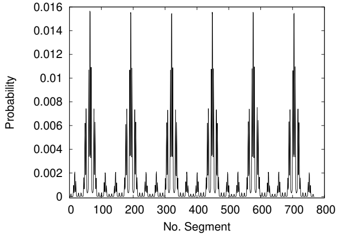
$r_i \neq \text{constant} \qquad \theta_i = \text{ran}(0, 2\pi)$

Find maximal radius and Jump uniformly.



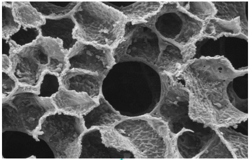
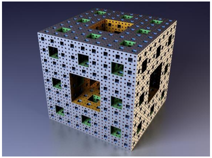
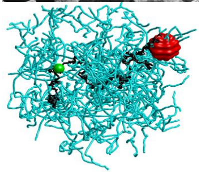
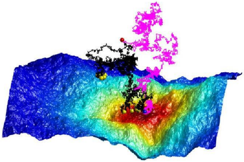
Compute distribution probability on each segment:

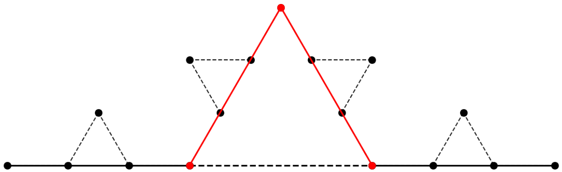




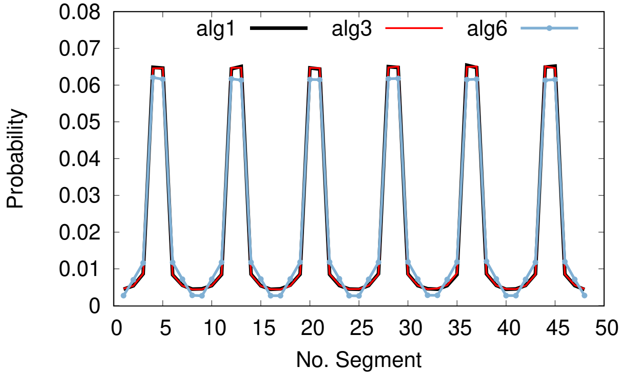
D. S. Grebenkov, et al. Physical Review E, 71(5), 056121 (2005).

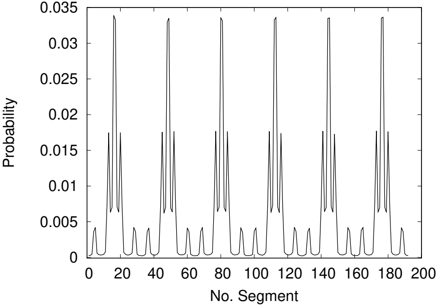
Thanks for your attention!

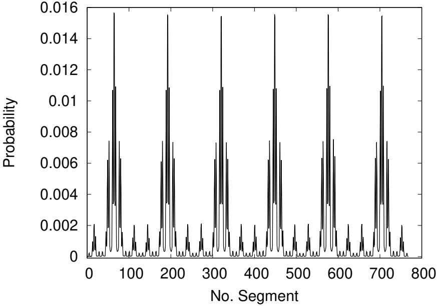





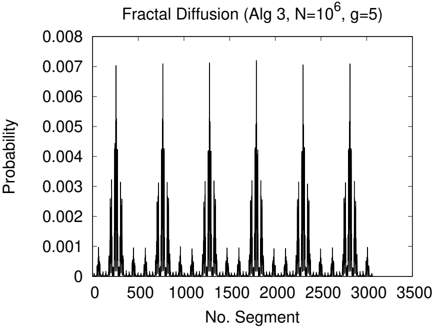


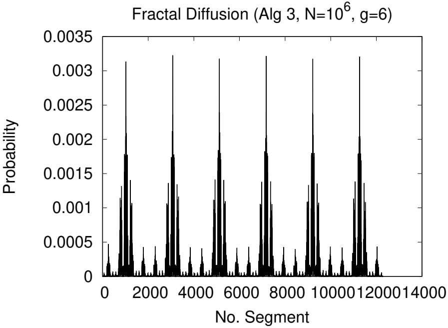
$$P\left(\vdots\right) \neq \sum P(|)$$




Probability
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0 20 40 60 80 100 120 140 160 180 200
No. Segment


Probability
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
0 100 200 300 400 500 600 700 800
No. Segment


Fractal Diffusion (Alg 3, N=10^6, g=5)
Probability
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
0 500 1000 1500 2000 2500 3000 3500
No. Segment


Fractal Diffusion (Alg 3, N=10^6, g=6)
Probability
0.0035
0.003
0.0025
0.002
0.0015
0.001
0.0005
0
0 2000 4000 6000 8000 10000 12000 14000
No. Segment

Local Time ℓ

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

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

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