Master 2: *Physics of Complex Systems*

INTERNSHIP PROPOSAL

Laboratory name: **Laboratory of Condensed Matter Physics**
CNRS identification code: **UMR7643**
Internship director'surname: **Denis GREBENKOV**
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Internship location: **Laboratory of Condensed Matter Physics, Ecole Polytechnique, Palaiseau, France**
Thesis possibility after internship: YES
Funding: NO (but it is possible to apply for a scholarship from Ecole Polytechnique)

Probabilistic and spectral insights onto diffusion-controlled reactions

Diffusion-mediated surface phenomena are crucial for human life and industry, with examples ranging from oxygen capture by lung alveolar surface to heterogeneous catalysis, gene regulation, membrane permeation, and filtration processes. A novel probabilistic approach based on the concept of boundary local time has been recently proposed to investigate the intricate dynamics of diffusing particles near a reactive surface [1,2]. In contrast to conventional descriptions based on the Fokker-Planck (e.g., Laplace) operator, the spectral formulation of the proposed approach relies on another, less common pseudo-differential operator. This general formalism allows one to describe new surface reaction mechanisms and to model various natural phenomena in physics, chemistry and biology. The disentanglement of the geometric structure of the medium from surface reactivity opens far-reaching perspectives for modeling, optimization, and control of diffusion-mediated surface phenomena.

The goal of the internship (and of the forthcoming PhD thesis) consists in elaborating this original approach in several complementary directions: (i) a more general mathematical formulation; (ii) the development of efficient numerical methods for calculating spectral properties of the governing operator in complex media; (iii) the analysis of new mechanisms for surface reaction with variable, encounter-dependent reactivity; and (iv) applications of the new theory in chemistry and biology such as search for partially reactive targets, distribution of the first-passage times for multiple "impatient" particles (with eventual dissociation from the target), diffusion in dynamic heterogeneous media or search for diffusing targets [3].

The candidate is expected to have a solid background in theoretical/mathematical physics or applied mathematics, be skilled in numerical simulations (e.g., in Matlab) and motivated for interdisciplinary research across mathematics, physics, chemistry and biology. The internship can potentially be continued as a PhD thesis under the condition of obtaining a PhD scholarship (in order to be able to apply for such a scholarship at Ecole Polytechnique, the candidate should have excellent notes).

Bibliography

[1] D. S. Grebenkov, Paradigm Shift in Diffusion-Mediated Surface Phenomena, Phys. Rev. Lett. **125**, 078102 (2020) [online: https://pmc.polytechnique.fr/pagesperso/dg/publi/2020_06.pdf]

[2] D. S. Grebenkov, *Spectral theory of imperfect diffusion-controlled reactions on heterogeneous catalytic surfaces*, J. Chem. Phys. **151**, 104108 (2019) [online: https://pmc.polytechnique.fr/pagesperso/dg/publi/2019_15.pdf]

[3] Y. Lanoiselée, N. Moutal, and D. S. Grebenkov, *Diffusion-limited reactions in dynamic heterogeneous media* Nature Comm. **9**, 4398 (2018) [online: https://pmc.polytechnique.fr/pagesperso/dg/publi/2018_10.pdf]