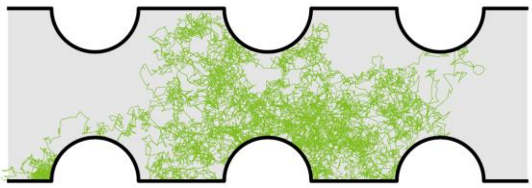
Master 2 Internship

Title: Dispersion in channels: the effect of surface mediated diffusion or time-dependent boundaries.

Supervisor: Thomas Guérin, David Dean

Contact: thomas.guerin@u-bordeaux.fr / david.dean@u-bordeaux.fr



Project: How fast does a cloud of tracer particles, moving stochastically in a complex heterogeneous medium, disperse? This question naturally appears in a wide range of contexts, including mixing, sorting, contaminant spreading or chemical reactions kinetics. At large length and time scales, dispersion is usually characterized by an effective diffusion tensor whose components can be considerably different from typical microscopic diffusivities. In particular, the problem of reduction of diffusivity in channels with non-uniform cross-section has received a lot of attention. So far, most of existing theories consider only the case of particles moving in channels with impenetrable and fixed boundaries. However, in many cases, the situation can be more complex: the local diffusivity is in general decreased at the vicinity of a boundary, which can also be attractive and/or fluctuate with time.

Recently **[1,2]**, we have obtained general formulas that enable to calculate the effective diffusivity in general heterogeneous media. Here, we wish to extend these formulas to cover the case of surface mediated diffusion and/or fluctuating boundaries to enable the understanding of these problems analytically. We expect non-trivial effects to arise: for example, in the case of dilute spheres, it is known that attractive boundaries can (under some conditions) lead to an increase of effective diffusivity – a seemingly counter-intuitive effect, since one should expect a decrease of diffusivity associated to the trapping on obstacles **[3]**. We will determine whether this effect still exists in channels. During this **theoretical** internship, the student will address these problems with analytical methods (based on stochastic differential equations, Fokker-Planck equations) that will be completed with numerical simulations.

Refs. **[1]** Guérin, T., & Dean, D. S. Force-induced dispersion in heterogeneous media. *Physical review letters*, ***115***, 020601 (2015).
[2] Mangeat, M., Guérin, T., & Dean, D. S. Geometry controlled dispersion in periodic corrugated channels. *Europhysics Letters*, ***118,*** 40004 (2017).
[3] Putzel, G. G., Tagliazucchi, M., & Szleifer, I. (2014). Nonmonotonic diffusion of particles among larger attractive crowding spheres. *Physical review letters*, ***113***, 138302 (2014).