

Finding saddle points of energy landscapes: why and how?

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One approach to bridging the gap between fully atomistic models and more coarse-grained descriptions is to use Markov State Models parameterized by the Eyring–Kramers formulas. These formulas provide the transition rates between local minima of the potential energy function and require the identification of both local minima and saddle points. This methodology is, for instance, employed in materials science, particularly in kinetic Monte Carlo models.

In this talk, I will first present a recent result obtained in collaboration with D. Le Peutrec (Université de Nantes) and B. Nectoux (Université Clermont Auvergne), which establishes the mathematical foundations of this approach by deriving the Eyring–Kramers exit rates from the overdamped Langevin dynamics [LLPN25]. I will then introduce a recent algorithm, developed jointly with P. Parpas (Imperial College London), for locating saddle points [LP24]. I will explain how both of these works rely on the concentration properties of the eigenvectors of Witten Laplacians in the low-temperature regime.

References

- [LLPN25] T. Lelièvre, D. Le Peutrec, and B. Nectoux. Eyring-kramers exit rates for the overdamped langevin dynamics: the case with saddle points on the boundary. *Journal de l'Ecole Polytechnique*, 12:881–982, 2025.
- [LP24] T. Lelièvre and P. Parpas. Using witten laplacians to locate index-1 saddle points. *SIAM Journal of Scientific Computing*, 46(2):A770–A797, 2024.