Variables collectives et modèles génératifs pour l'échantillonnage de systèmes métastables

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Deep generative models parametrize very flexible families of distributions able to fit complicated datasets of images or text. These models provide independent samples from complex high-distributions at negligible costs. On the other hand, sampling exactly a target distribution, such as the Boltzmann distribution of a physical system, is typically challenging : either because of dimensionality, multi-modality, ill-conditioning or a combination of the previous. A recent line of work using generative models to accelerate sampling has shown promises but still struggles as the system size gets large. In this talk, I will discuss an approach tackling this challenge by using a generative model to explore the configuration space of a collective-variable (CV) and a non-equilibrium candidate Monte Carlo to recover an unbiased all-atoms configurations. The approach revisits CV-guided sampling with two main advantages. Firstly, the collection of CVs need not be restricted to a few variables and can include tens or hundreds of degrees of freedom. Secondly, updates in the CV space are non-local thanks to the generative model, leading to a fast exploration regardless of free energy barriers. This talk is based on [1].

[1] C. Schönle, M. Gabrié, T. Lelièvre, G. Stoltz. *Sampling metastable systems using collective variables and Jarzynski–Crooks paths.* Journal of Computational Physics, **527**, 113806, 2025. doi : 10.1016/j.jcp.2025.113806.

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