Dynamics and long-time state prediction by generative models (2-year Postdoc - Open until filled, starting date in 2026)

Motivation: Molecular Dynamics (MD) algorithms are one of the most widely used techniques in computational physics, chemistry, and biology. These simulations involve solving a large number of Newton's equations, which is computationally intensive and prone to numerical instabilities. Recently, several approaches have been investigated in order to accelerate molecular dynamics simulations using machine learning [1, 2]. Machine learning (ML) techniques, such as Support Vector Machines (SVM), Multi-Layer Perceptrons (MLP), and Graph Neural Networks (GNN), have been increasingly used to forecast future dynamics from static configurations. While these models achieve remarkable accuracy, they often function as complex "black boxes", offering little insight into the underlying mechanisms and the reason for high performance. To address this limitation, the field of interpretable machine learning has emerged, aiming to enhance the transparency and trustworthiness of ML models by explaining their predictions.

Goal: Our goal is to develop a surrogate model that replaces solving Newton's equations with machine learning, in particular in the field of glassy dynamics [3]. In particular, we plan to tackle the following challenges:

- How to robustly predict future dynamics based on the initial configuration while bypassing costly computations?
- How can the outcome of the prediction and its performance be interpreted?

Environment: The candidate will join the Université Clermont-Auvergne at the Laboratoire de Mathématiques Blaise Pascal (UMR 6620) and will be part of the Cluster IA MIAI chair *R-GAINS*. This project aims to establish an interdisciplinary task force dedicated to developing robust AI-enhanced probabilistic sampling methods to accelerate the simulation of high-dimensional complex systems, particularly those involving high-energy barriers or rare-event phenomena. The work spans multiple scales, from short-term dynamics to long-time behavior and equilibrium states, and brings together advances in generative modeling, machine learning, Monte Carlo methods, and rigorous mathematical analysis. The project will be supervised locally by Alain Dequidt (UCA, ICCF), Arnaud Guillin (UCA, LMBP) and Manon Michel (CNRS, LMBP). Importantly, the postdoc is expected to work across both Clermont-Ferrand and Grenoble (LIPhY, Vivien Lecomte and Misaki Ozawa), with regular visits to each site, in order to benefit from the complementary expertise of the two hubs. Finally, the candidate will be integrated into the broader research ecosystem of the MIAI (Multidisciplinary Institute in Artificial Intelligence) Cluster, which fosters cutting-edge AI research and its applications across scientific domains.

Profile: We are looking for a motivated candidate with a background in probability, statistical physics, or computational physics or chemistry, and an experience in generative modeling and stochastic processes. Programming experience is required. For more details, contact Manon Michel (manon.michel@uca.fr). Applications should come with CV, cover letter, short research statement and reference contacts.

Webpages:
R-GAINS chair webpage: https://https://r-gains.pages.math.cnrs.fr/website/
MIAI's webpage: https://miai.univ-grenoble-alpes.fr/

References:

[1] Sharma, Anand, Chen Liu, and Misaki Ozawa. *Selecting relevant structural features for glassy dynamics by information imbalance*, *International Conference on Learning Representations*, The Journal of Chemical Physics 161.18, 2024.

[2] G.-M. Cherchi, A. Dequidt, A. Guillin, N. Martzel, P. Hauret, and V. Barra. *ML GLE: A Machine Learning Enhanced Generalized Langevin Equation Framework for Transient Anomalous Diffusion in Polymer Dynamics*, J. Comput. Phys. 514, 113210, 2024.

[3] Jung, G., Alkemade, R.M., Bapst, V. et al. *Roadmap on machine learning glassy dynamics*, Nat Rev Phys 7, 91–104 (2025).