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S E M I N A I R E

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" Toward General, Reliable and Reactive Machine-Learning Potentials using Force-Field-enhanced Neural Networks "

Machine-learning (ML) potentials have recently proven to be a powerful alternative to force fields (FF) for the simulation of complex chemical systems. The data-driven approach facilitates the parameterization of the models and enables the accurate reconstruction of ab-initio potential energy surfaces. Most current ML approaches however rely on local atomic descriptors, thus neglecting long-range interactions that are crucial for the simulation of large condensed-phase and biophysical systems.
To resolve this issue, we couple ML and FF in the framework of Force-field-Enhanced Neural Network Interactions (FENNIX). This approach leverages state-of-the-art equivariant neural networks to predict local energy contributions and multiple atom-in-molecule properties which are then used as geometry-dependent parameters for well-chosen force-field terms that account for long-range interactions. While being trained only on small organic molecules and multimers, FENNIX produces stable condensed-phase Molecular Dynamics simulations -- including nuclear quantum effects -- and predicts accurate liquid water properties. Preliminary results on solvated alanine dipeptide and small proteins show that Force-field-enhanced neural networks open a promising route toward high-precision reactive dynamics of biological systems.

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14h00

Salle des conférences