Προτεινόμενα Θέματα Διπλωματικής Εργασίας

Από

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Α. Αξιοποίηση τεχνητής νοημοσύνης για την εκτίμηση δυναμικών πεδίων σε μοριακές προσομοιώσεις

Συνοπτική περιγραφή (στα αγγλικά):

Polymeric systems are complex materials of great technological importance, in manufacturing, packaging, and for environmental applications. They are particularly challenging to study with molecular simulations, which is a powerful technique to investigate at the molecular level the properties of complex chemical systems, but it is extremely computationally intensive. Multiscale simulation strategies are thus required for polymer systems, that are usually elaborate and system-specific. These schemes could be generalized and streamlined by the application of Machine Learning (ML) methods.

A main advantage of ML models in the context of molecular simulations is that they are not constrained to a predefined mathematical function, therefore they are endowed with higher flexibility and expressive character compared to traditional molecular models. Recently, neural networks have shown great promise in the development of improved atomistic force fields.

In the overarching project into which the work will be integrated, we investigate the use of Machine Learning methods (including deep learning alternatives) to create optimized molecular force fields, using suitable descriptors for the local environment. The obtained potential will be integrated into a Molecular Dynamics open-source software (LAMMPS) to perform large-scale molecular simulations. Finally, we aim to create an automated pipeline for the evaluation of the Machine Learned force field against structural and thermodynamic properties of the systems.

The project involves a synergy of Software and Knowledge Engineering Lab (SKEL | The AI lab) of the Institute of Informatics Telecommunications and the Molecular Thermodynamics and Modeling of Materials Laboratory (MTMML) of the Institute

of Nanoscience and Nanotechnology.

Related literature:

1. Husic, B. E.; Charron, N. E.; Lemm, D.; Wang, J.; Pérez, A.; Majewski, M.; Krämer, A.; Chen, Y.; Olsson, S.; De Fabritiis, G.; Noé, F.; Clementi, C. Coarse Graining Molecular Dynamics with Graph Neural Networks. J. Chem. Phys. 2020, 153 (19). https://doi.org/10.1063/5.0026133

2. Doerr, S.; Majewski, M.; Pérez, A.; Krämer, A.; Clementi, C.; Noe, F.; Giorgino, T.; De Fabritiis, G. TorchMD: A Deep Learning Framework for Molecular Simulations. J. Chem. Theory Comput. 2021, 17 (4), 2355–2363. https://doi.org/10.1021/acs.jctc.0c01343