Master thesis proposal

Hybrid Machine Learning Models for Molecular Dynamics simulations of material properties

Keywords : physically recurrent neural networks; materials science; molecular dynamics; surrogate modelling

SCIENTIFIC DESCRIPTION :

Molecular Dynamics (MD) simulations are ubiquitous in physics, chemistry and more predominantly material science, being responsible for one of the largest consumptions of computational time on supercomputers worldwide. Their resolution is associated with the size and the vibration frequency of atoms (Å and fs), scales usually inaccessible by experiments. Yet, by essence this resolution limits the scales that can be tackled with MD. Extending accessible scales has been an ongoing challenge for decades. One way to reach higher scales in materials science simulations is by linking lower-scale MD models to upper-scale continuum models [1, 2]. Still, although they allow higher scales to be reached, these approaches still entail a large number of expensive MD simulations that can take months to run. Machine learning techniques are therefore seen as the missing link in these multiscale approaches, by building fast and accurate surrogate models to take the place of expensive MD simulations. Yet, even though a wide range of machine learning surrogates have been proposed for multiscale modeling of materials [3], conventional machine learning models relying purely on data-driven mechanisms still require an inordinate amount of computationally expensive training data in order to be useful, largely defeating their intended purpose. We propose a novel approach to tackle this issue by embedding small but fully-fledged MD simulations in neural network architectures, inspired by recent advances in multiscale modeling of materials. With this proposal we instead draw inspiration from Physically Recurrent Neural Networks (PRNNs), a recently-proposed hybrid surrogate model combining neural network architectures with purely physics-based models for material behavior (Fig. 1c). The core of the approach is to embed intact physical models in neural network architectures and let the network both decide the inputs of the physical models as well as how to combine their outputs. This makes the approach rather unique with respect to popular ways to combine physics with machine learning: physical constraints come directly from the embedded models and are satisfied by construction (in contrast to PINNs [8]) and the AI part of the model not only decides how physical models are combined but also plays a role in model building by deciding what inputs will be passed to them (in contrast to Mixture-of-Expert models). PRNNs already deliver impressive performance with simple embedded models (elastic springs, plasticity models) making multiscale simulations run up to 10000× faster and learn with up to 100× less data than conventional models (Fig. 1b). But up until now they have never been used to embed more complex (and powerful) numerical models.

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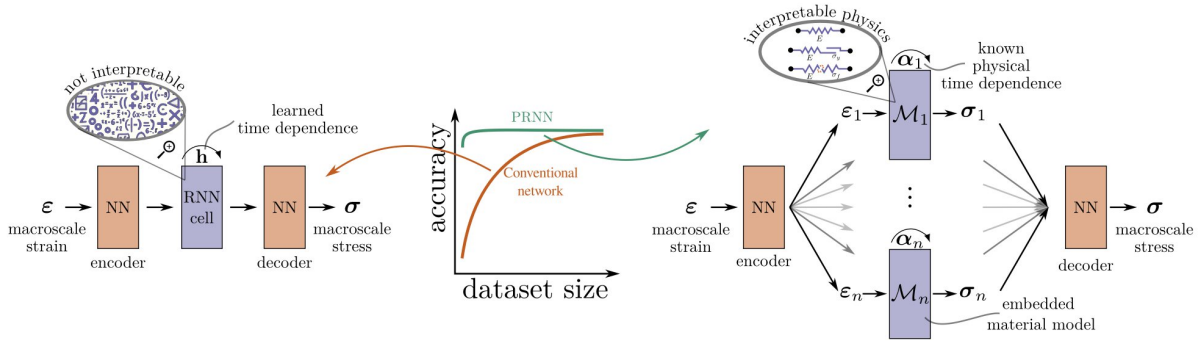

(a) conventional ML surrogate (b) training data requirements (c) Physically Recurrent Neural Network

Figure 1: Physically Recurrent Neural Networks (PRNNs) applied for multiscale material behavior simulations.

The student will join a collaboration between two groups located in Rennes (France) and Delft (The Netherlands), with expertise in molecular dynamics for the simulation of the mechanical properties of amorphous materials and expertise in surrogate modelling of the constitutive behaviour of materials using PRNNs, respectively.

[1] M. Vassaux, R. A. Richardson, and P. V. Coveney. The heterogeneous multiscale method applied to inelastic polymer mechanics. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 377(2142):20180150, February 2019.
[2] M. Vassaux, S. Wan, W. Edeling, and P. V. Coveney. Ensembles Are Required to Handle Aleatoric and Parametric Uncertainty in Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 17(8):5187–5197, August 2021.
[3] B. A. Le, J. Yvonnet, and Q.-C. He. Computational homogenization of nonlinear elastic materials using neural networks. International Journal for Numerical Methods in Engineering, 104(12):1061–1084, 2015.

Techniques/methods in use : The project will imply the use of Python and associated libraries. In particular, pyTorch for the implementation of the PRNNs and TorchMD for the implementation of the small molecular dynamics models.

Applicant skills : The applicant is expected to have a generic knowledge in machine learning as well as skills in Python; knowledge in materials science and skills in pyTorch would be a plus.

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