Machine learning-enhanced material dynamics simulations using generative methods integrated with experimental data for applications in Energy and Drug Discovery

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1. Introduction

Machine learning is transforming scientific research by accelerating and enhancing traditional methodologies. This shift is particularly impactful in materials science, where understanding material properties and optimizing manufacturing processes have long been challenging. Machine learning techniques now enable faster discoveries, more accurate predictions, and better-informed decision-making [1].

In the field of energy materials and drug discovery—the primary research focus of the innovation network ARTEMIS *("Artificial Intelligence Powered Material Design"*) at TUM — this technological shift is especially impactful, as material properties play a crucial role in determining performance. Here, I will examine the application of generative models in enhancing the speed and accuracy of numerical simulations for exploring material properties for different applications, with an emphasis on dynamical properties. These models not only accelerate simulations by identifying key internal dynamical degrees of freedom [2] but also enable the construction of faster surrogate dynamics.

Furthermore, I will discuss how machine learning is being utilized to analyze experimental data [3, 4] and integrate it with numerical simulations.

2. Method

2.1 Identification of Collective Variables for Dynamical Systems using Variational Autoencoders

Collective Variables (CV) of a dynamic system can be interpreted in many ways. Two of the most common interpretation are of the variables expanding the high variance degrees of freedom and that which expand the slowest evolving degrees of freedom. Under the assumption of ergodicity, the two become equivalent. In the context of coarse-grained dynamics of a system, CVs allow for retention of the maximum amount of information for a given degree of coarsening. This is applicable to different scales of dynamics and has been used extensively to accelerate molecular dynamics (MD) simulations [6] with hand-crafted CVs and more recently CVs learned through machine learning methods. By using the disentangled latent space of a β-Variational Autoencoders (β-VAEs) instead of normal autoencoders, we can benefit from the regularization effect for information retention capability as well as interpretability of the model.

We previously applied machine learning methods in an unsupervised framework to elucidate the dynamics of a host-guest system. We recently used the β-VAEs in an iteratively explore the configuration space of molecular systems. We show that the regularization due to the β parameter leads to the CVs becoming orthogonal to each other and maximizes the information retention capability of the model. This also increases the probability that a single CV corresponds to a single geometric feature of the structure which we can detect by performing a correlation analysis with a set of geometric variables.

Similarly, for development of a surrogate model for dynamics of materials, CVs can be used as course-grain dimensions to reduce the computational effort of simulating many degrees of freedom in time. This leads to a loss in information but if the CVs are so constructed that slow degrees of freedom that they capture correspond to the timescale of the dynamics of interest, the dynamics is accelerated with minimal loss of relevant information.

2.1 Learn a Surrogate Dynamics using Temporal Fusion Transformers

An excellent surrogate model is the so-called Temporal Fusion Transformer (TFT) model. This model, introduced in [5] possessed many unique properties that make it eminently suitable for capturing the dynamic behavior of a system as well as shed light to the parameters of relevance for every case. In particular, the unique combination of Long Short-Term Memory (LSTM) networks [7] and transformers [8]. LSTMs allow for the capturing of short-term dependencies. In contrast the transformers are responsible for capturing long time range phenomena. This is of crucial importance in dynamical systems that contain rare and far between events that still affect the overall dynamics. Additionally, the gated mechanisms and the introduction of simulation parameters through static covariates allows for an inbuilt feature importance. As example we can reference the investigation of Solid-State Electrolyte depletion layer formation. Through our model we not only successfully predicted the ion evolution, but we also determined the relative relevance of the bias, permittivity and ion concentration on the material bulk.

Lastly, TFT allows for future covariates as well as past. This has multiple uses. Firstly, in cases such as a temperature affected phenomenon, we can create

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predictions for variable defined temperature at will. Further, in cases where we possess multiple levels of theory, the prediction of the highest accuracy can further be informed by the phenomenon propagation as determined by a coarser simulation.

2.3 Application

Concretely, to demonstrate the principle, we have applied the model to different case studies, including for drug discovery to study drug/target interactions [2], or to optimize materials for energy production. As an example, the case of a supercapacitor with solid-state electrolyte (SSE), described in [9,10] in detail, was selected. The model describes the formation of a space charge layer at the electrode when an external voltage is applied (the charging process). The numerical model to describe the process is based on kinetic Monte Carlo [11]. The mobile ions are described like particle that can move under the external effect of a voltage from one ionic vacancy to a neighbor one. This process is described using hopping transport. The different vacancies have different energies, which modulates the hopping rate[10]. Moreover, the ions can interact not just with the external field, but also with each other via Coulomb interaction, making the problem a concrete many-body challenge. Thanks to the TFT characteristics, we can introduce side information in terms of experimental data, like permittivity and external voltage. In figure 1, it is shown that not only we can accurately predict the phenomenon evolution, even for relatively computationally expensive simulation parameters, but we can also reconstruct the kinetic Monte Carlo derived uncertainty field. This is crucially of high importance as the dynamics alone are not a full reflection and adequate representation of the KMC capabilities.

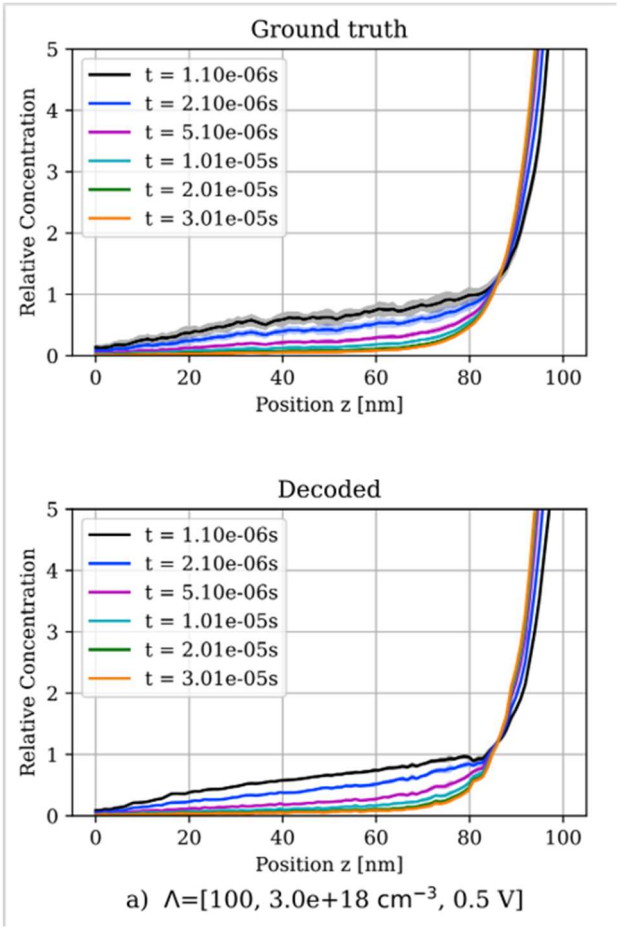

Fig. 1: Transient at the cathode of the supercapacitor with SSE. The profile shows the normalized ionic density as a function of time (t). This is a simulation with permittivity 100, equilibrium ionic density $3x10^{18}$ cm^{-3} and 0.5 Volt applied. Top: kMC simulation. Bottom: TFT prediction.

2.4 Conclusions

In the present proceeding, we have demonstrated the use of machine learning architecture to generate surrogate dynamics, including the effects of experimental parameters. This integration establishes a unified data stream, offering a comprehensive perspective on material performance by bridging simulated predictions with real-world observations. The ultimate objective is to streamline the research workflow—from simulation to experimentation [5]—minimizing the time and resources needed to design, test, and optimize novel materials. By harnessing machine learning to expedite these processes, we can significantly shorten the development cycle of advanced materials, driving innovation in energy, medical technologies, and beyond.

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