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DECTRIS

ARINA with NOVENA

Fast 4D STEM



DECTRIS NOVENA and CoM analysis of a magnetic sample.

Sample courtesy: Dr. Christian Liebscher, Max-Planck-Institut für Eisenforschung GmbH.
Experiment courtesy: Dr. Mingjun Wu and Dr. Philipp Reis, Friedrich-Alexander-Universität, Erlangen-Nürnberg.

Meeting-report

Learning the Physics of Liquid Phase TEM Nanoparticle Trajectories Using Physics-Informed Generative AI

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Visualizing and characterizing the diffusion of single nanoparticles in various chemical and biological environments enables us to infer the underlying material properties of the environment. The advent of liquid phase transmission electron microscopy (LPTEM) has introduced a novel avenue for high spatial and temporal resolution single particle tracking at the nanoscale, enabling us to investigate diffusion dynamics at a scale inaccessible before [1-4]. Understanding and interpreting the underlying physics of single nanoparticle trajectories has traditionally been approached with canonical statistical methods such as time-averaged mean squared displacement. However, these methods fail on single short trajectories, especially the ones with non-gaussian and non-ergodic characteristics – common features of LPTEM trajectories. These challenges have led to a body of computational research on classifying short single particle trajectories into classes of anomalous diffusion and determining their anomalous diffusion exponents (α) using supervised machine learning and deep learning models that are trained on simulated trajectories with known α [5-7]. This problem has also been handled with unsupervised deep learning approaches to learn the properties of simulated trajectories of known diffusion classes but without labels of physical parameters like α [8, 9]. However, experimental data from single particle tracking experiments remains a largely unknown mixture of different anomalous diffusion classes with unknown diffusion parameters, making it difficult to classify them into ideal stochastic models. Furthermore, learning the dynamics of real experimental nanoparticle trajectories is a crucial step in advancing electron microscopy into the space of fully automated workflows.

Here, we have leveraged the generative power of AI models to learn the physics of real trajectories obtained from LPTEM movies and generate synthetic single particle trajectories. To this end, we have developed a generative physics-informed transformer-based variational autoencoder that is trained on a large data set of experimental trajectories, mixed with some simulated trajectories, of gold nanorods from LPTEM experiments. LPTEM experiments were carried out with gold nanorods dispersed in water on a Tecnai F30 TEM with an accelerating voltage of 200 kV using a Poseidon LPTEM holder. The movies were collected using the Gatan Oneview camera and processed using a thresholding-based algorithm to extract the coordinates of the gold nanorods at each movie frame. Using the powerful self-attention mechanism of transformers that has shown remarkable results in learning the underlying correlations in sequence-based data, this model learns the time-dependent dynamics of the experimental trajectories in its continuous latent space representation based on statistical/physical properties. We demonstrate that our model can separate trajectories into different diffusion classes and recognize the differences in their statistical properties. More importantly, our model can be used as a black-box simulator for generating synthetic single-particle trajectories from LPTEM. The latter is an extremely useful feature in that it generates an unlimited number of trajectories for downstream tasks, e.g., in developing an AI-based workflow for automating in situ electron microscopy experiments.

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