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# Fourier–Thermodynamic Latent Modeling for Temperature-Dependent Plasma Mixing

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**Jannik Eisenlohr**

Department of Computational Mathematics, Science and Engineering  
Michigan State University  
East Lansing, MI 48824  
eisenl10@msu.edu

**Youngsoo Choi**

Center for Applied Scientific Computing  
Lawrence Livermore National Laboratory  
Livermore, Ca 94550  
choi15@llnl.gov

**Michael Murillo**

Department of Computational Mathematics, Science and Engineering  
Michigan State University  
East Lansing, MI 48824  
murillom@msu.edu

## Abstract

We present FT-LaSDI (Fourier Thermodynamics-based Latent Space Dynamics Identification), a three-stage reduced-order modeling (ROM) framework for temperature-dependent mixing in quantum-statistical MD of carbon–hydrogen plasmas. Using Sarkas with the Deutsch quantum statistical potential, we train on selected temperatures and evaluate both training-rollout fidelity and interpolation. On training temperatures, forecasting errors remain below 1% for the first half of the trajectory and rise to  $\sim 10\%$  by the final timestep; interpolation at 7.5 eV is not yet successful (relative error  $> 50\%$ ). Inference with FT-LaSDI yields an estimated speed-up of **500 $\times$**  over full MD per trajectory, with a one-time training cost of **24** GPU-hours. This study highlights the promise of thermodynamically consistent ROMs for MD-driven plasma dynamics and pinpoints loss weighting, optimizer choice, and batch size as key levers for robust interpolation.

## 1 Introduction

Reduced-order models (ROMs) that preserve physical structure are increasingly important for accelerating high-fidelity simulations in computational physics. Classical ROM approaches such as proper orthogonal decomposition (POD), dynamic mode decomposition (DMD), and Galerkin projection have proven effective for many continuum problems, but they often struggle with systems that exhibit strong nonlinearities, non-equilibrium behavior, or thermodynamic constraints. These challenges have motivated machine-learning-based ROMs that explicitly encode conservation laws and entropy dynamics.

Thermodynamically consistent approaches such as GENERIC Formalism-Informed Neural Networks (GFINNs) [8] and their parametric extension pGFINNs [3] embed the GENERIC framework directly

into latent neural dynamics, ensuring energy conservation and non-decreasing entropy. While these models have shown strong performance on canonical PDEs, applications to particle-based quantum-statistical molecular dynamics (MD) remain limited.

Fourier-domain methods have recently gained prominence in operator learning—most notably Fourier Neural Operators (FNOs) [4], which use spectral convolution layers to efficiently capture parametric PDE behavior. Although designed for continuum fields, their success highlights the advantages of spectral representations for extracting dominant physical modes. This motivates our use of Fourier projections to obtain low-variance, physics-aware features from noisy MD particle data.

In this work, we develop FT-LaSDI, a Fourier- and thermodynamics-based latent modeling framework for temperature-dependent mixing in carbon–hydrogen plasmas simulated with Sarkas [1] using the Deutsch quantum statistical potential [5]. These quantum-statistical MD simulations provide a challenging testbed due to short-range correlations, temperature sensitivity, and microscopic noise. FT-LaSDI smooths particle data, projects fields onto low-dimensional Fourier coefficients, compresses them with an autoencoder, and evolves latent states using pGFINN dynamics that enforce GENERIC degeneracy conditions.

Our study focuses on two questions: (i) how accurately FT-LaSDI can reconstruct and forecast MD trajectories at training temperatures, and (ii) whether the learned latent dynamics interpolate to intermediate temperatures. While training performance is strong, interpolation to 7.5 eV is not yet successful, revealing sensitivities to loss weighting, optimizer choice, and latent dimensionality and pointing to important directions for refinement.

**Contributions.** (1) Extension of thermodynamically consistent latent-dynamics models to quantum-statistical MD of C/H plasmas with QSP interactions. (2) A Fourier-based feature pipeline, inspired in part by spectral operator-learning approaches such as FNOs, enabling low-noise compression of MD fields. (3) An empirical evaluation demonstrating accurate training reconstructions and forecasts, along with a detailed analysis of interpolation failures and associated sensitivities.

## 2 Background

### 2.1 GENERIC Formalism

The GENERIC framework (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) [2, 6] expresses dynamics as

$$\dot{z} = L(z) \frac{\partial E}{\partial z} + M(z) \frac{\partial S}{\partial z}, \quad (1)$$

where  $L$  is a skew-symmetric Poisson operator and  $M$  is a symmetric positive semi-definite friction operator. The degeneracy conditions,

$$L(z) \frac{\partial S}{\partial z} = 0, \quad M(z) \frac{\partial E}{\partial z} = 0,$$

ensure energy conservation ( $\dot{E} = 0$ ) and entropy production ( $\dot{S} \geq 0$ ), encoding the first and second laws of thermodynamics [8].

### 2.2 pGFINNs and Latent Dynamics

GFINNs embed the GENERIC structure into neural networks by parameterizing  $E$ ,  $S$ ,  $L$ , and  $M$  with architectures that satisfy the required degeneracy conditions [8]. The parametric extension, pGFINNs, integrates parameter dependence directly into the latent dynamics, enabling interpolation across physical parameters such as Reynolds number or plasma temperature [3].

Recent work on tLaSDI (thermodynamically consistent latent dynamics identification) further introduced Jacobian-based regularization for improved generalization [7], which we incorporate here.

### 2.3 Method overview: FT-LaSDI pipeline

FT-LaSDI comprises three stages: (1) **Fourier projection**. Using periodic boundaries, we Gaussian-smooth particle data to construct 1D density and velocity fields and project them to Fourier space, yielding spectral coefficients; (2) **Autoencoder reduction**. A fully connected encoder–decoder

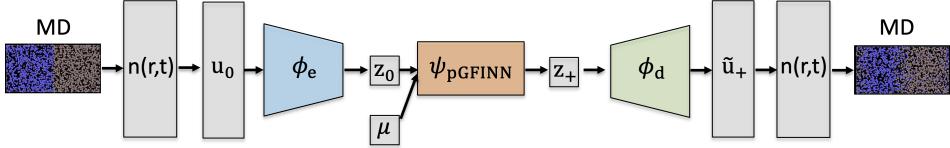


Figure 1: Schematic of the FT-LaSDI framework. Raw particle data is coarse-grained into density/velocity fields  $n(r, t)$  /  $n_v(r, t)$  compressed via Fourier transform into  $u$ , reduced through an autoencoder, and evolved in latent space with parametric GENERIC Formalism-informed Neural Networks (pGFNNs).

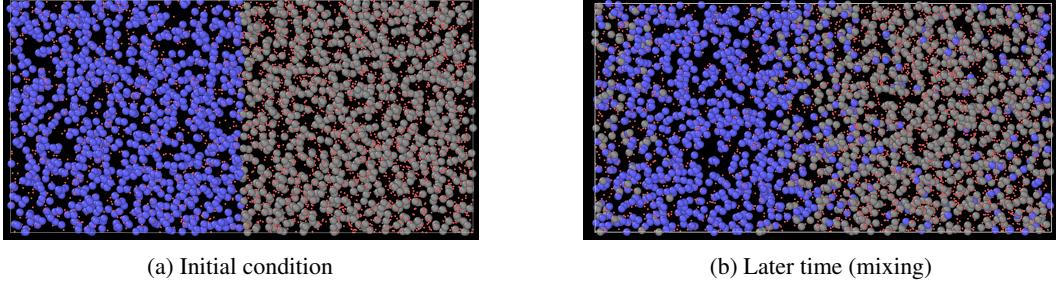


Figure 2: Sarkas MD snapshots for the C/H plasma with explicit electrons and Deutsch QSP. (a) Initial configuration with randomized positions and temperature-set velocities. (b) Later-time state indicating spatial mixing.

(width decreasing approximately linearly to a latent dimension) compresses the spectral state to a low-dimensional latent variable  $z$ . (3) **Thermodynamic latent dynamics (pGFNN)**. The latent time evolution is learned under GENERIC constraints (skew-symmetric  $L$ , symmetric PSD  $M$ , degeneracy conditions), ensuring energy conservation and nondecreasing entropy.

#### 2.4 Sarkas MD Setup

We employed the Python-based MD package *Sarkas* [1] to simulate binary carbon–hydrogen plasmas with explicit electrons. Ion-ion interactions were modeled using the *Deutsch potential* [5], a QSP that regularizes the short-range Coulomb divergence by accounting for quantum diffraction (finite electron thermal de Broglie wavelength), thereby preventing unphysical close encounters while retaining classical long-range behavior.

Each simulation contained  $N_C = N_H = 1000$  ions with periodic boundary conditions. To isolate the effect of temperature, the initial particle positions were kept identical across simulations, while the initial velocities were rescaled to match the target thermal energy. Simulations were performed at  $T \in \{5, 7.5, 10, 12.5, 15\}$  eV, each spanning 1000 timesteps.

Figures 2a–b show snapshots of the MD system at initialization and a later time, respectively, illustrating the emergence of spatial mixing from microscopic particle motion.

#### 2.5 Fourier Projection of Fields

From the particle trajectories, we compute the one-dimensional number density  $n(x, t)$  and velocity density  $nv(x, t)$ . We restrict the analysis to the 1D direction along which mixing develops, since this captures the dominant large-scale dynamics of interest. Because this raw molecular dynamics data still contains strong microscopic fluctuations, we first map the discrete particle positions onto a uniform spatial grid using a Gaussian kernel density estimation (KDE) procedure. Each particle contributes a unit-mass Gaussian profile centered at its instantaneous position,

$$W(x - x_i; \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{x - x_i}{\sigma}\right)^2\right], \quad (2)$$

where  $\sigma$  controls the effective smoothing width. This normalized kernel ensures that each particle contributes equally to the overall density while suppressing high-frequency noise. The velocity density is calculated using the same kernel, except that the contribution of each particle is weighted by its instantaneous velocity rather than unit mass. In this work,  $\sigma$  was chosen to be one-tenth of the shortest domain dimension, corresponding approximately to the average interparticle spacing in that direction.

The smoothed density and velocity-density fields are then evaluated on a uniform grid and transformed to Fourier space via a discrete Fourier transform (DFT), yielding complex mode coefficients  $a_k(t)$ . For input to neural networks, we truncate to the lowest 50 modes for each of the four fields (number and velocity densities for carbon and hydrogen), and divide the complex coefficients into their real and imaginary parts, resulting in  $4 \times 50 \times 2 = 400$  input channels per time snapshot. This choice of 50 modes was determined empirically: inverse FFT reconstructions using this cutoff reproduced the smoothed fields with less than 1% relative error, indicating that the retained modes capture the dominant spectral content of the mixing dynamics.

## 2.6 Autoencoder Architecture

The Fourier-projected state at each timestep (400 real-valued inputs) is compressed using a fully connected autoencoder. We conducted a sweep over architectures ranging from 2 to 6 hidden layers, latent dimensions from 2 to 20, and activation functions including `tanh`, `elu`, and `relu`. Across these configurations, we found that a three-layer encoder–decoder with `tanh` activations and a latent dimension of  $n_z = 6$  provided the most stable training behavior and the lowest reconstruction error.

The encoder reduces the 400-dimensional spectral state to the latent variable  $z \in \mathbb{R}^6$ , and the decoder mirrors this structure to reconstruct the Fourier coefficients. Deeper or wider networks did not improve accuracy and often introduced training instability, while smaller latent dimensions failed to capture the nonlinear spectral correlations induced by mixing. With the chosen architecture, the autoencoder achieves reconstruction errors on the order of  $10^{-4}$  across training temperatures, ensuring that the latent space retains the essential large-scale spectral features required for the downstream pGFINN latent-dynamics model.

## 3 Results and Discussion

### 3.1 Training Performance and Loss Convergence

The model was trained on Sarkas MD trajectories at temperatures  $\mu \in \{5, 10\}$  eV, with interpolation targeted at the unseen  $\mu = 7.5$  eV.

The training loss converged to  $\sim 10^{-4}$  reconstruction error on the autoencoder, indicating near-perfect compression of Fourier modes. The trajectory loss stabilized around  $10^{-5}$ , showing that the latent GENERIC dynamics were able to evolve the compressed state stably over long time horizons.

AdamW provided better stability and generalization than SOAP, although SOAP achieved lower final training losses. Contrary to previous work on thermodynamically consistent latent dynamics [3], large batch sizes ( $\geq 500$ ) did not achieve convergence during training. Instead, smaller batch sizes were critical for stable convergence, as one example shown in Fig. 3a demonstrates.

### 3.2 Interpolation at 7.5 eV

At present, the model does not yet successfully interpolate the dynamics at  $\mu = 7.5$  eV. Predictions diverge from the ground truth Fourier mode trajectories, with errors accumulating rapidly after a few timesteps. Consistent with this divergence, the relative error exceeds 50 % across modes, indicating that the current model does not achieve meaningful interpolation. This reflects the sensitivity of the latent GENERIC dynamics to hyperparameter tuning, especially in the balance between reconstruction and Jacobian regularization terms.

We are nonetheless confident that with improved loss balancing, deeper autoencoder architectures, and possibly hybrid optimizer strategies, the FT-LaSDI ROM framework will achieve accurate interpolation. Prior work on PDE benchmarks with tLaSDI and pGFINNs suggests that interpolation in parameter space is a natural strength of the approach [7, 3].

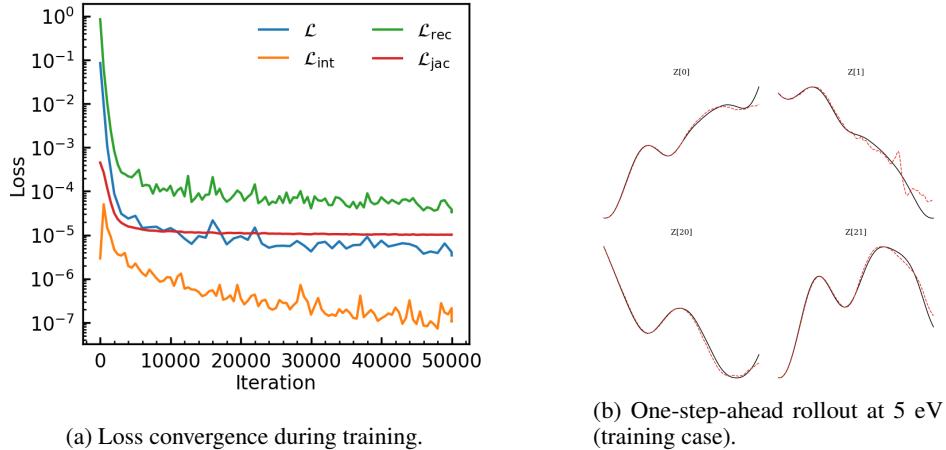


Figure 3: (a) Training loss convergence. (b) Forecasting performance on training data.

### 3.3 Forecasting on Training Data (5 eV)

To evaluate fidelity in the training regime, we examined one-step-ahead forecasts starting from the initial conditions at  $\mu = 5$  eV. The model was able to roll forward accurately for the entire 1000 timesteps, reproducing the Fourier mode trajectories without significant phase error. Quantitatively, the relative error remains below 1 % for the first half of the trajectory and grows gradually to about 10 % by the final timestep. This confirms that the learned latent dynamics are consistent with the MD generator in the training regime.

### 3.4 Computational Speedup

A central motivation for reduced-order modeling is the dramatic reduction in computational cost relative to full molecular dynamics (MD) simulation. In our setting, one Sarkas simulation of a C/H plasma with  $N_C = N_H = 1000$  ions and 1000 timesteps requires approximately 12 CPU-hours on conventional HPC hardware. This cost is fixed per simulation regardless of how many Fourier modes or observables are later analyzed, since particle trajectories must be advanced at every timestep.

By contrast, once trained, our reduced-order model—consisting of Fourier projection, autoencoder compression, and pGFINN latent evolution—can roll out trajectories of equal length in only 120 seconds on GPU. The majority of this cost arises from the latent ODE integration, with Fourier transforms and autoencoder operations contributing negligible overhead.

This corresponds to a speedup factor on the order of  $10^2$ – $10^3$ , depending on hardware. Importantly, this speedup is reported at the full-simulation level rather than per-trajectory: while MD simulations are inherently fixed-cost runs, the surrogate can generate temperature-dependent forecasts essentially instantaneously once trained. These gains highlight the potential of thermodynamically consistent reduced-order models to bridge expensive MD simulations and fast surrogate dynamics.

## 4 Conclusion

We demonstrated that FT-LaSDI ROM, constrained by the GENERIC formalism, can learn temperature-dependent latent dynamics from quantum-statistical MD of C/H plasmas using Gaussian-smoothed, Fourier-projected fields. On training temperatures, the surrogate achieves near-perfect reconstruction and accurate forecasting. Interpolation to the intermediate temperature (7.5 eV), however, currently fails: rollouts diverge with large relative error, pointing to sensitivity in loss balancing, optimizer choice, and batch size. These results highlight both the promise of thermodynamically consistent surrogates for MD-driven plasma dynamics and the need for targeted refinements to realize robust interpolation across temperature.

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