Learning non-equilibrium mesoscopic dynamics with Onsager principle

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1. Introduction

Discovering governing equations from data is a central challenge in scientific computing. While black-box deep learning models such as Neural ODEs and Fourier Neural Operators (FNOs) [1] achieve strong predictive performance, they often lack physical interpretability and long-term stability, frequently violating conservation laws or exhibiting nonphysical energy growth beyond the training horizon.

Structured learning approaches mitigate these issues by embedding physical principles into network architectures. In particular, OnsagerNet [2, 3] enforces thermodynamic consistency by decomposing dynamics into dissipative and conservative components under the Generalized Onsager Principle. However, extending this framework to infinite-dimensional dynamics remains challenging due to the prohibitive dimensionality of spatial discretization and the lack of structure preservation in standard operator learning methods.

To address these limitations, we propose Spectral OnsagerNet, a novel operator-learning framework that preserves thermodynamic structure in function space. For periodic systems, we represent dissipative and conservative operators directly in the spectral domain, enabling efficient parameterization of the energy functional and transport operators in Fourier space. This design combines the computational efficiency of spectral methods with the stability guarantees of the Onsager principle, facilitating data-driven discovery of PDE dynamics that are both physically interpretable and intrinsically stable.

2. Method

We propose a general data-driven framework for learning mesoscopic dissipative dynamical systems from observational data. Given discrete spatio-temporal observations of a mesoscopic field, $u(t,x)$, we seek to infer its governing evolution equation in a data-driven manner. Our approach is grounded in nonequilibrium thermodynamics and assumes that the dynamics follow a generalized Onsager principle, namely

$$\partial_t u = -\left[\mathcal{M}(u) + \mathcal{W}(u)\right] \frac{\delta V(u)}{\delta u}. \tag{1}$$

where the dissipative operator $\mathcal{M}(u)$ is symmetric and positive semi-definite, and the conservative operator $\mathcal{W}(u)$ is skew-symmetric. Consequently, the energy $V(u)$ is non-increasing along trajectories, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t} V(u(t)) \leq 0. \tag{2}$$

2.1 Structure-preserving parameterization of the dissipative and conservative operator

We focus on systems satisfying translational invariance, implying that the operators $\mathcal{M}$ and $\mathcal{W}$ act as convolutions in the physical domain. We next set $\Omega = \mathbb{T}^d$ and apply the Fourier transform to both sides of eq. (1). The convolution theorem implies that eq. (1) is equivalent in Fourier space to

$$\begin{aligned} \partial_t \hat{u}^{[k]} &= -\left[\hat{K}_{\mathcal{M}}(u)^{[k]} + \hat{K}_{\mathcal{W}}(u)^{[k]}\right] \hat{\mu}_t^{[k]}, \\ \hat{\mu}_t^{[k]} &= \mathcal{F}\left[\frac{\delta V_2}{\delta u}\right]^{[k]}, \quad k = 0, 1, \cdots, \end{aligned} \tag{3}$$

where we denote by $\mathcal{F}$ the Fourier transformation on $L^2(\Omega)$. We then introduce a simple yet effective parameterization that preserves the symmetry and positive semi-definiteness of the dissipative operator, as well as the skew-symmetry of the conservative operator:

$$\begin{aligned} \hat{K}_{\mathcal{M}}(u) &= \Re\left(G_\psi(\hat{u})\right)^2, \\ \hat{K}_{\mathcal{W}}(u) &= \mathrm{i}\Im\left(G_\psi(\hat{u})\right). \end{aligned} \tag{4}$$

Here, we use $\Re(\cdot)$ and $\Im(\cdot)$ to denote the real and imaginary parts of the complex-valued network output $G_\psi(\hat{u})$.

2.2 Parameterization of the energy functional

We decompose V into three parts to account for point-wise, local, and global interactions. More specifically, we take the ansatz

$$V(u) = \underbrace{\int_\Omega \left[\frac{\alpha}{2}|u|^2 + F(u(x))\right] \mathrm{d}x}_{V_0(u)} + \underbrace{\int_\Omega \frac{\beta}{2}|\nabla u|^2 \mathrm{d}x}_{V_1(u)} + V_2(u)$$

with positive trainable scalars α and β, where $V_2 : \mathcal{X} \to \mathbb{R}$ is a functional capturing the residuals of the integrands. It follows that the Fourier series of the functional derivative is given by

$$\hat{\mu}_t^{[k]} = \left[\alpha + (2\pi k)^2 \beta\right] \hat{u}^{[k]} + \mathcal{F}\left[F'(u)\right]^{[k]} + \overline{\frac{\partial v_2}{\partial \hat{u}^{[k]}}}. \tag{5}$$

We thus use $v_\theta : \ell^2 \to \mathbb{R}$ to approximate v_2 with a proper truncation m on the infinite-dimensional space ℓ^2.

2.3 Existence and uniqueness of the solution

Theorem. Under mild assumptions, the dynamics eq. (1) admits a unique solution in the solution space

$$W(0,T;\mathcal{X}) := \{u \in L(0,T;\mathcal{X}) \mid \partial_t u \in L(0,T;\mathcal{X})\} \tag{6}$$

for any finite time T, where $\mathcal{X} = H^1(\Omega)$.

3. Numerical results

3.1 *Training and the baselines*

The reference solution is obtained via highly accurate numerical schemes, and the training is based on coarse sampling across the time axis. We compare our model with the following baselines.

Ground Truth (abbreviated as GT) We use the real $\mathcal{M}$, $\mathcal{W}$, and the energy V, and apply the explicit forward Euler numerical stepper. Since the numerical stepper differs from that used for generating the reference trajectories, the error essentially captures the discrepancy imposed by the numerical schemes.

Residual OnsagerNet (abbreviated as Res-OnsagerNet) The last gradient term is parameterized by a vector-valued network. This is the most naive approach to learning the increment in the spectral space; however, the parameterization for the term μ_t is not guaranteed to be a functional derivative.

Fourier Neural Operator (abbreviated as FNO) We use the FNO architecture [1] to directly learn the dynamics in the physical space, which serves as a robust baseline in the field of operator learning.

Spectral OnsagerNet (our work, abbreviated as S-OnsagerNet) We apply the parameterization described in the previous section. We also evaluate a variant where the energy V is fixed to the ground truth for comparison.

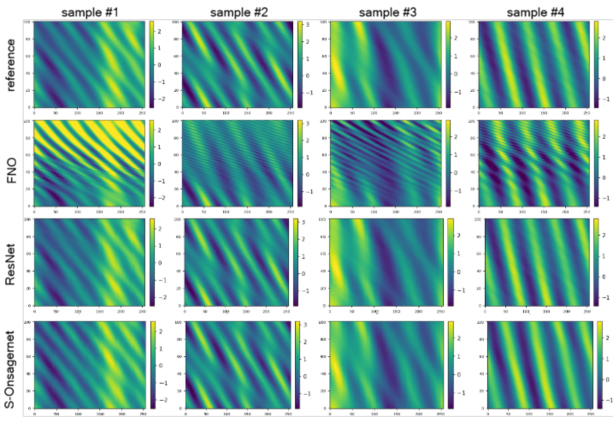

Fig. 1: Comparison of predictions on the KdV dataset.

model	Allen-Cahn	KdV
GT (real $\mathcal{M}$, $\mathcal{W}$, and V)	7.59e-4	1.19e-3
FNO[1]	5.28e-6	1.31e-3
Res-OnsagerNet	6.02e-4	1.34e-3
S-OnsagerNet w/ real V	7.58e-4	7.17e-5
S-OnsagerNet	**6.43e-7**	**7.30e-5**

Table 1: Prediction error (↓) for various baselines

3.2 *Experimental results*

First, in terms of prediction capability, Spectral OnsagerNet achieves the highest accuracy among all tested baselines, including Residual OnsagerNet and the Fourier Neural Operator (FNO). This validates that enforcing physical structure—specifically the symmetry of dissipation and skew-symmetry of conservation—serves as a strong inductive bias that enhances generalization in data-driven modeling.

Besides, our model exhibits a unique ability to bridge the gap between continuous physics and discrete observations. Notably, Spectral OnsagerNet outperforms the "Ground Truth" baseline, which couples the exact physical operators with a standard explicit numerical stepper. This suggests that our learned operators can implicitly compensate for the discretization errors inherent in numerical schemes. Consequently, our framework offers a promising solution for exploring microscopic dynamics using macroscopic data, effectively correcting for the discrepancies introduced by finite time-stepping.

Finally, unlike black-box surrogates, our approach offers significant interpretability. By explicitly parameterizing the system dynamics through the energy functional $V(u)$, Spectral OnsagerNet allows us to recover and analyze the underlying potential of the system. This transparency enables the discovery of governing physical laws rather than merely fitting trajectories, marking a step forward in robust, physically interpretable scientific machine learning.

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