OnsagerFlow: Learning mesoscopic dynamics from microscopic simulation

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1. Introduction: Microscopic to Mesoscopic

The goal of this work is to develop a systematic framework for bridging physical systems from the microscopic to the mesoscopic scale through coarse-graining. Consider the Ising model: a microscopic simulation with 16384×16384 spins is computationally expensive. By contrast, coarse-graining the microscopic spins yields a mesoscopic description on a much smaller grid (e.g., 128×128). Enabling simulations directly at this mesoscopic level, therefore, allows access to system sizes that are orders of magnitude larger.

Motivation: Learn mesoscopic dynamics from microscopic simulations with three key advantages:

1. **Large-Scale Simulation**: Mesoscopic models enable simulations at scales inaccessible to microscopic methods.
2. **First-Principle Accuracy**: Unlike deterministic PDEs (e.g., Allen–Cahn) that rely on many assumptions, our approach achieves quantitative consistency with microscopic data.
3. **Physical Structures**: The learned model preserves interpretable physical quantities, mobility K, free energy $\mathcal{F}$, and interaction kernel $\mathcal{J}$, rather than being a black-box neural network.

1.1 Coarse Graining: Problem Definition

We start from the Ising model with Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i. \tag{1}$$

To describe the system at mesoscopic scales, we introduce a coarse-grained magnetization field obtained by block averaging microscopic spins:

$$m^L(t, \mathbf{x}) = \frac{1}{B^d} \sum_{z \in \Lambda_B(\mathbf{x})} \sigma_t(z), \tag{2}$$

where $\Lambda_B(\mathbf{x})$ denotes a block of linear size B centered at $\mathbf{x}$, and B^d is the block volume. This field captures local magnetization fluctuations while smoothing out microscopic spin noise.

1.2 Limitations of Traditional Deterministic PDEs[1]

In the hydrodynamic limit, the mesoscopic field converges to a deterministic evolution equation of nonlocal mean-field type[2]:

$$\partial_t m(x,t) = -m(x,t) + \tanh\Big(\beta\big[(\mathcal{J} * m)(x,t) + h(x)\big]\Big), \tag{3}$$

where $\mathcal{J}$ is the interaction kernel inherited from the microscopic coupling.

When $\mathcal{J}$ is short-ranged and sufficiently smooth, a local approximation leads to the Allen–Cahn equation,

$$\partial_t m = \kappa \Delta m - f(m) + \beta h, \qquad f(m) = rm + um^3, \tag{4}$$

which is widely used as an effective macroscopic model for phase separation dynamics.

However, both descriptions are inherently deterministic and describe only the typical evolution of the coarse-grained field. As a result, they fail to capture fluctuation-driven phenomena such as metastable transitions and rare magnetization flips that remain relevant at mesoscopic scales.

These deterministic PDEs have two major limitations: (1) they involve *too many assumptions* on functional forms (tanh, $1 - m^2$ mobility, local $\mathcal{J}$), making them **not quantitatively accurate**; (2) they *ignore stochastic fluctuations*, which are essential at the mesoscopic scale.

2. OnsagerFlow: A Stochastic PDE with FDT

2.1 The Onsager/FDT Framework

We propose a **stochastic PDE** that satisfies the **fluctuation-dissipation theorem (FDT)**[3]-a fundamental physical principle linking noise and dissipation:

$$\boxed{\partial_t m = -K(m) \frac{\delta \mathcal{F}}{\delta m}(m, \mathcal{J}) + \sqrt{2\beta^{-1}}\, B(m)\, \xi,} \tag{5}$$

with the **FDT constraint** $K(m) = B(m)^* B(m)$. Here $K(m) \geq 0$ is the mobility operator, $\mathcal{F}[m]$ is the free energy functional, ξ is space-time white noise, and $B(m)$ is the noise amplitude. The FDT ensures that drift and noise are *coupled* through the same mobility K, guaranteeing thermodynamic consistency.

The free energy functional has the form:

$$\mathcal{F}[m] = \int \frac{1}{\beta} s(m)\, dx - \frac{1}{2} \iint \mathcal{J}(x-y) m(x) m(y)\, dx\, dy - \int hm\, dx, \tag{6}$$

with variational derivative:

$$\frac{\delta \mathcal{F}}{\delta m}(x) = s'(m(x)) - (\widehat{\mathcal{J}} * m)(x) - h. \tag{7}$$

Key insight: The SPDE *structure* (gradient flow + FDT) is dictated by physics (detailed balance at microscopic level). But the *functions* ($K(m)$, $s'(m)$, $\mathcal{J}$) should be learned from data, not assumed with human-imposed approximations.

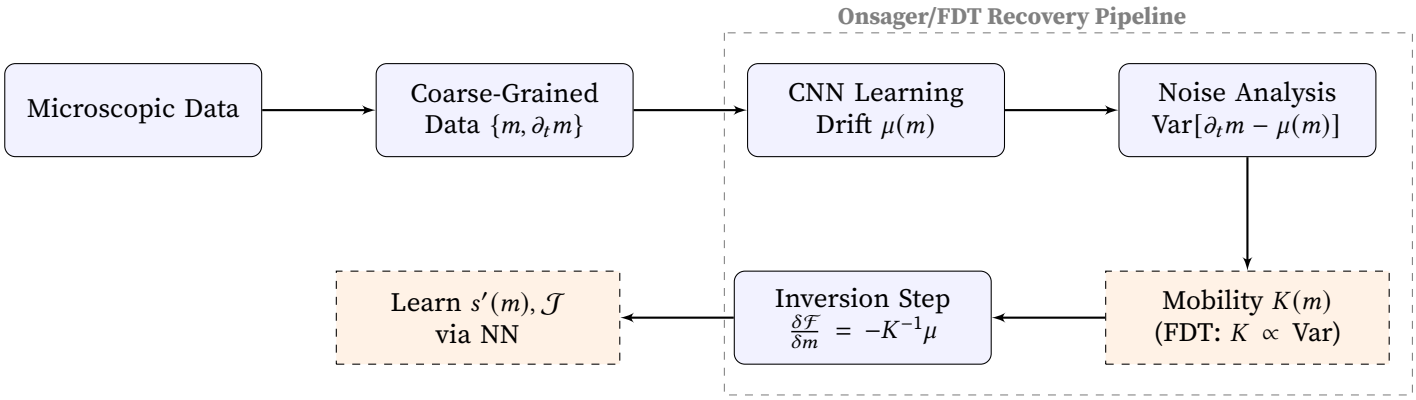

Fig. 1: Full-width architecture of the OnsagerFlow pipeline, illustrating the path from raw data to learned physical components.

2.2 Data-Driven Learning of Physical Components

We use neural networks to learn the three key components from first-principle microscopic simulation data:

1. Mobility $K(m,T)$: Traditional approaches assume K is constant (high-T) or $K(m) = 1-m^2$ (low-T)—neither aligns with data. We learn the true $K(m,T)$ directly using the FDT relation: $K \propto \mathrm{Var}[\partial_t m \mid m]$.

2. Free Energy Derivative $s'(m)$: Instead of assuming $s'(m) = \mathrm{arctanh}(m)$, we parameterize it with neural networks and fit from data.

3. Interaction Kernel $\mathcal{J}$: Instead of assuming local or mean-field forms, we learn the full nonlocal kernel by solving a linear inverse problem.

3. Results and Applications

Comparison of mesoscopic approaches:

- **Hydrodynamic limit / Allen–Cahn**: Deterministic PDE, assumed functions → *Not accurate*
- **Micromagnetic LLG**: Deterministic PDE, assumed functions → *Not accurate*
- **Ours (OnsagerFlow)**: SPDE with FDT + learned functions → *Principled and accurate!*

We validate on the 2D Ising model with Kac-type interactions, accurately recovering mobility and interaction kernels. The framework extends to atomistic spin dynamics (ASD) and Mumax3 simulations, bridging the gap between experimental scales (~20 μm) and current simulation capabilities (~400 nm).

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