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# Deep Learning-Based Computational Method for Soft Matter Dynamics: Deep Onsager-Machlup Method

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**Abstract.** A deep learning-based computational method is proposed for soft matter dynamics – the deep Onsager-Machlup method (DOMM). It combines the brute forces of deep neural networks (DNNs) with the fundamental physics principle – Onsager-Machlup variational principle (OMVP). In the DOMM, the trial solution to the dynamics is constructed by DNNs that allow us to explore a rich and complex set of admissible functions. It outperforms the Ritz-type variational method where one has to impose carefully-chosen trial functions. This capability endows the DOMM with the potential to solve rather complex problems in soft matter dynamics that involve multiple physics with multiple slow variables, multiple scales, and multiple dissipative processes. Actually, the DOMM can be regarded as an extension of the deep Ritz method (DRM) developed by E and Yu that uses DNNs to solve static problems in physics. In this work, as the first step, we focus on the validation of the DOMM as a useful computational method by using it to solve several typical soft matter dynamic problems: particle diffusion in dilute solutions, and two-phase dynamics with and without hydrodynamics. The predicted results agree very well with the analytical solution or numerical solution from traditional computational methods. These results show the accuracy and convergence of DOMM and justify it as an alternative computational method for solving soft matter dynamics.

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## 1 Introduction

Approximate variational methods such as the Ritz-type method have been widely used to study the structure, phase behaviors, and dynamics of soft matter [1–4]. These methods are mostly based on the following variational principles: the variational principle of minimum free energy (MFEVP) [1,2,4], Onsager's variational principle (OVP) [5–7], and the Onsager-Machlup variational principle (OMVP) [3,8]. In these variational methods, some trial functions to the problem are assumed empirically where the state variables are taken as combinations of some analytical functions with a much smaller number of adjustable parameters [4,7,9,10]. Such methods simplify the problem significantly: they bypass the derivation and solution of the complicated governing differential equations and go directly from the variational statement to an approximate solution to the problem.

Recently, it has been proposed that the power of these variational methods can be further enhanced if we use deep neural networks (DNNs) to construct the trial functions. For example, the deep Ritz method (DRM) [11] uses variational formulations of physics models (for example from MFEVP) to solve static problems in physics. In our former work [10], we have applied DRM to the spontaneous bending of active elastic solids. Actually, DRM is regarded as one of the DNN methods for solving partial differential equations (PDEs). Among other DNN methods, the most popular methods are the Physics-Informed Neural Network (PINN) [12] and its variants [13] where the residual of a PDE is minimized as a loss function. Another type of DNNs for the approximate solutions of PDEs is the data-driven approach. It involves collecting a large amount of data under similar conditions for the same PDE to learn a solution operator that directly maps the conditions of the PDE to its solution. Examples of such methods include Deep Operator Neural Network (DeepONet) [14], Fourier Neural Operator (FNO) [15], OnsagerNet [16], Variational Onsager Neural Networks (VONNs) [17], flow maps [18], and many others. The main difference between the data-driven approach and the mechanism-driven approach is that the mechanism-driven does not require data and can be treated similarly to those in traditional methods. All these deep learning methods have recently been used in many different problems in soft matter physics, prediction of microphase-separated structures in diblock colpolymers [19], stochastic control of colloidal self-assembly [20], phase separation dynamics [21], bubble growth dynamics [22]. For more discussions and applications about DNNs for solving PDEs, we recommend the review paper by Karniadakis *et al.* [13].

Here we are particularly interested in deep-learning methods for solving PDEs such as DRM that combine variational principles with deep learning. Recently several differ-