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On Diffusion-based Graph Neural Networks for Lagrangian Fluid Simulations

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Abstract

Machine learning surrogates have become ubiquitous in scientific applications, extending or replacing components of traditional simulators. In particular, diffusion-based approaches have been gaining traction in both Eulerian and Lagrangian ML, with random-walk noise being a typical choice to train particle-based CFD surrogates [1]. This study investigates two recent diffusion-based refinement strategies, PDE-Refiner [2] and Autoregressive Conditional Diffusion Models [3], adapted to improving the particle distribution of reverse Pouiselle flow and lid-driven cavity simulations. These datasets were introduced in the LagrangeBench paper [4] and are generated by the JAX-SPH in-house particle-based differentiable solver [5]. Evaluation metrics extend beyond positional errors to encompass kinetic energy and Sinkhorn distance, the latter of which is directly related to the particle distribution we want to improve with diffusion. However, our empirical results suggest that neither of the two advanced diffusion approaches offers an empirical advantage over using random-walk noise to corrupt particle positions. In contrast, simple random-walk noise is more efficient in terms of both accuracy and inference speed.

Keywords: Lagrangian, smoothed particle hydrodynamics, graph neural networks, diffusion.

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