Physics-Corrected Graph Network Simulators (GNS) for Modelling Fluid Flow

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ABSTRACT

Recent advancements in machine learning, particularly deep learning, have significantly impacted fluid dynamics simulation. Graph Network Simulators (GNS) have become a powerful tool for modelling complex particle-based fluid flows. These models leverage graph structures to capture the relationships between particles, making them effective for representing fluid particle interactions. The strength of this method lies in its ability to train fluid particles to learn physics in a controlled lab environment and to apply this knowledge in real-world out-of-distribution (OOD) scenarios.

The GNS code, alongside the *WaterRamps* dataset and *WaterVortex* example, is available on GitHub [1]. However, despite their successes, GNS models face challenges in handling boundary conditions, such as inlet velocity, and in generalising to (OOD) scenarios. To address these challenges, we introduce the Particle Trickle Release (PTR) algorithm, enabling accurate implementation of inlet velocity boundary conditions in GNS models. The PTR algorithm uses a binomial distribution to account for inflow velocity and boundary length, ensuring more precise particle inflows. Additionally, we compare sequential training with the widely used dynamics bootstrapping method to improve GNS models' capacity to generalise fluid dynamics.

Our findings reveal that in OOD scenarios, the GNS algorithm fails to conserve volume. To address this issue, we correct particle positions as an initial step to enforce incompressibility, followed by calculating the velocity divergence to evaluate the particles' ability to learn incompressibility constraints. We also discuss the limitations of GNS techniques, highlight their advantages over Physics-Informed Neural Networks (PINNs), and outline future research directions to further enhance fluid dynamics modelling using GNS.

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REFERENCES

[1] https://github.com/google-deepmind/deepmind-research/tree/master/learning_to_simulate.