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Enhancing Data-Assimilation in CFD using Graph Neural Networks

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Introduction

The fusion of **Computational Fluid Mechanics** (CFD) with **Machine Learning** (ML) algorithms is providing a promising approach to face the traditional time-consuming and computational demanding challenges in CFD simulations. In our work, we propose an adjoint based optimization method augmented by a **Graph Neural Network** (GNN) in a CFD **data assimilation** problem of a flow passing by a bluff body.

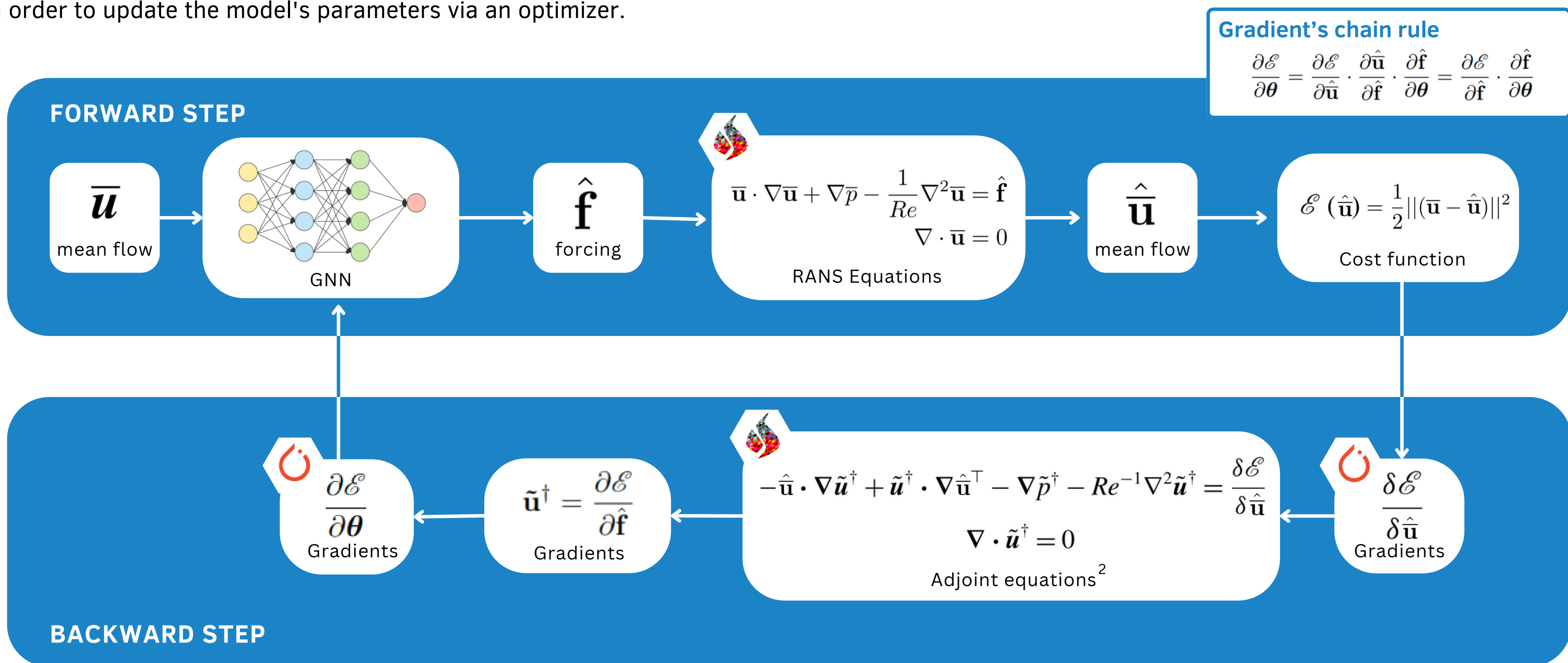
Our approach involves an end-to-end process, where a GNN model is employed to predict the closure term for the **Reynolds-Averaged Navier-Stokes Equations** (RANS). The equations are used as part of the architecture to constrain physical consistency in the GNN prediction¹.

Augmented training loop

The complete end-to-end⁴ training loop can be formulated as follows:

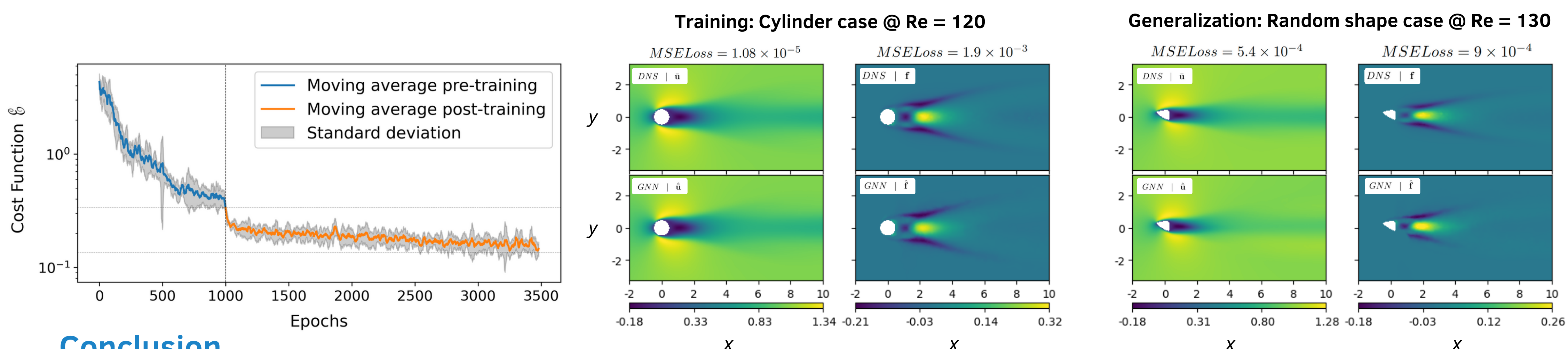
Forward step: the corrupted or incomplete mean flow field is propagated through the GNN model. The model generates an initial prediction for the RANS closure term that, while potentially accurate, may lack physical coherence. These initial predictions are used in a FEM solver to obtain the corresponding mean flow as solution of the RANS equations. A cost function is defined minimizing the difference between the latter and the mean flow computed by means of **Direct Numerical Simulation** (DNS).

Backward step: Gradients of the cost function are back-propagated through the adjoint equations and gathered with the gradients from the GNN through the gradient's **chain-rule** in order to update the model's parameters via an optimizer.



Results

The **proof of concept** of our approach on a **complete mean flow reconstruction** shows that the GNN model is **consistently learning** from this schema, thus demonstrating the correct inclusion of the RANS equations into the GNN model. The GNN pre-training phase has been performed in a supervised fashion by using only the time averaged flow of a cylinder at Reynolds number $Re = 120$ as input and its relative forcing stress as target. The **generalization capabilities** of this model on never seen cases, $O(10^{-4})$ on the MSELoss for random shaped bluff bodies, are far beyond the ones from a GNN model which learns exclusively from data⁵.



Conclusion

In this work, we introduced a novel algorithm for **data-assimilation** of a flow passing by a bluff body, combining the versatility of GNN with a FEM solver. An interface between the GNN model and the FEM solver enables communication between the two computational environments for a robust back-propagation of gradients during the training phase. The resulting data-assimilation scheme provides an appropriate **reconstruction of the mean flow**, relying on a pre-trained GNN model and keeping the **physical coherence** of the prediction through the constraint provided by the RANS equations. We are currently moving to **corrupted or incomplete mean flow reconstruction** and refining the technique for enhancing the generalization properties over unseen cases, including different geometries and flow parameters.

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