Internship Research Project - Master or Engineering degree
Graph Neural Networks for Fluid Mechanics Modelling

Key words : Deep Learning, Navier Stokes equations, Computational Fluid Dynamics (CFD), Hybrid Simulation.

Applications of CFD : Aerospace and Aerodynamics, Energy, Transportation, Weather Simulation, Fluid Flow, Heat Transfer...

INFORMATION

Profile : Bac+5 with a background in Computer Science / Physics / Applied Mathematics / Statistics / Signal
Company: Extrality, in cooperation with Machine Learning and Information Access team (MLIA) - Sorbonne University - https://mlia.lip6.fr
Starting date: Late February- April for 6 months
Location: Paris
Advantages: 50% on Navigo subscription, lunch tickets with Swile and salary : global package 1500 €
Contact: Contact jointly research@extrality.ai and patrick.gallinari@sorbonne-universite.fr with [**Internship Research Project : Extrality - MLIA/LIP6**] in the subject

1 Context

Conception of industrial products like cars, planes, rockets, wind turbines, boats... required to be tested in a virtual world instead of building a costly and dangerous prototype. These process and tools are called numerical simulations. Especially the step of product design in a fluid is called CFD (*Computational Fluid Dynamics*).

Traditional CFD frameworks rely on the power of intensive parallel computations to simulate the physical environments and to analyze fluid flow problems. The latter takes advantage of high speed computers. But despite the efficiency of existing tools, deterministic solutions are computationally expensive and could last several months to recover an approximate solution. This is due to the complexity of solving deterministically the Navier-Stokes equation, a PDE (*Partial Differential Equation*) governing the problem. But huge quantity of data extracted from numerical simulation solutions are today available to assess a new way to recover flow solutions. Deep Neural Networks (DNN) enjoy lots of success in different neighboring tasks, ranging from computer vision to speech recognition. Deep Learning is particularly interesting thanks to its universal approximation properties; capable at approximating any differentiable functions with respect to some regularity properties. Therefore, Deep Learning can be explored to solve CFD problems.

This promising new research trend is aimed at analyzing and controlling DNNs by taking advantage of the rich background of CFD numerical analysis. This research topic has gained a lot of interest in the Machine Learning and Physics scientific field. PDE and machine learning offer complementary strengths : the modeling power and interpretability of differential equations and as mentioned the generalization power of deep neural networks.

1.1 Purpose of the internship

The goal of this internship is to develop Deep Learning models for numerical simulation. A promising way will be to study Geometric Deep Learning (spatial and spectral). These methods include the challenges in choosing appropriate convolutional and pooling operators, 3D mesh and graph representations, incorporating physical knowledge to deep learning models, multi-scale losses, SGD based physical constraints.

This internship allows you to be at the crossroad of industrial application with Extrality and research state of the art with the MLIA team (LIP6, Sorbonne Universités).

1.2 Outcome

Patents and/or publications in conferences/journals.

2 Extrality R&D

Extrality offers industrial design companies very fast numerical simulations thanks to Machine Learning. Concretely our SaaS platform and our tech enable our clients in aerospace, aeronautics, automotive, transport and energy to virtually test the physical properties of their designs, e.g. aerodynamics, up to 10000x times faster, leading to better lead time.

Our vision: empower engineers to focus on what really matters, i.e. creating disruptive products, instead of wasting their time on very long and tedious computations.

Extrality was founded by Pierre Yser (CTO), former Dassault Aviation Engineer and PhD in numerical simulations, and Nicolas Rasamimanana (CEO), tech entrepreneur with a PhD in Machine Learning. Extrality is based in Paris, with offices at Agoranov (Paris 6th).

The team is composed of top notch profiles, engineers and researchers, coming from the fields of aerospace industry, machine learning, and tech start-ups. Our team members have previously worked for successful ML companies, combining strong industrial profiles and academic excellence.

3 MLIA team/ Sorbonne University

MLIA - LIP6, Sorbonne University, is specialized on Statistical Machine Learning and Deep Learning. It is one of the foremost and pioneer groups in Deep Learning in France. Research ranges from algorithmic developments to application domains such as computer vision, natural language processing and complex data analysis. Under the direction of P. Gallinari, the group has started to develop 3 years ago a thematic on the modeling of dynamical physical systems with ML. This research direction has become a central topic of the team [2, 3, 4]. The team is involved in international and national academic collaborations and has developed a close cooperation with industrial R&D partners.

4 Desired profile

Background and skills to develop :

- Bac+5 with a background in Computer Science / Physics / Applied Mathematics / Statistics / Signal Processing
- Curious to open the deep learning black-box
- Interested by Computational Fluid Dynamics (CFDs) and numerical simulation
- Show enthusiasm to oscillate between fundamental and applied research
- Proficiency in Python for experimentation and data manipulation
- Strong knowledge of deep learning, machine learning and data mining
- Autonomy and initiative
- Demonstrable experience working on machine learning projects

- Great attention to detail and the ability to solve complex and cross disciplinary problems
- Passion for contributing to engineered products with AI to make a real impact
- Eager to learn : Numerical Analysis, Statistical Signal Processing, Computational Fluid Dynamics

Supervision :

1. **Academia** : Professor Patrick Gallinari (head of MLIA team).
2. **Extrality** research group : Pierre Yser (pierre@extrality.ai) doctor in Fluid Mechanics and Ahmed Mazari (ahmed@extrality.ai) doctor in deep learning

Spin off : possibility to pursue PHD studies within MLIA/LIP6 team (Sorbonne Universités, Campus Pierre et Marie Curie) and Extrality.

Working environment : Extrality is using cloud computation resources coming from different subcontractors. Deep Learning algorithms are developed in python using the Pytorch framework.

References

[1] Steven L. Brunton and Bernd R. Noack and Petros Koumoutsakos. Machine Learning for Fluid Mechanics. Annual Review of Fluid Mechanics, January 2020

[2] de Bezenac, E., Pajot, A. and Gallinari, P. 2018. Deep Learning For Physical Processes: Incorporating Prior Scientific Knowledge. ICLR (2018).

[3] Ayed, I., de Bezenac, E., Pajot, A. and Gallinari, P. 2020. Learning the Spatio-Temporal Dynamics of Physical Processes from Partial Observations. ICASSP (2020).

[4] Le Guen, V., Yin, Y., Dona, J., Ayed, I., de Bézenac, E., Thome, N. and Gallinari, P. 2021. Augmenting Physical Models with Deep Networks for Complex Dynamics Forecasting. http://arxiv.org/abs/2010.04456 (2021), 1–22.

[5] Kohl Georg Kiwon and Thuerey Nils. Learning Similarity Metrics for Numerical Simulations. In ICML, 2020

[6] Fourier Neural Operator for Parametric Partial Differential Equations. Submitted to ICLR, 2021

[7] Andreas Loukas. How hard is to distinguish graphs with graph neural networks? In NeurIPS, 2020

[8] Kim Byungsoo and C. Azevedo Vinicius and Thuerey Nils and Kim Theodore and Gross Markus and Solenthaler Barbara. Deep Fluids: A Generative Network for Parameterized Fluid Simulations. Computer Graphics Forum (Proc. Eurographics), 2019

[9] Andreas Loukas. What graph neural networks cannot learn: depth vs width. In ICLR, 2020

[10] P. R. Vlachas and J. Pathak and B. R. Hunt and T. P. Sapsis and M. Girvan and E. Ott and P. Koumoutsakos. Backpropagation algorithms and reservoir computing in recurrent neural networks for the forecasting of complex spatiotemporal dynamics. Neural Networks, vol. 126, pp. 191-217, 2020.

[11] Oyallon Edouard. Interferometric Graph Transform: a Deep Unsupervised Graph Representation. In ICML, 2020

[12] Dwivedi Vijay Prakash and Joshi Chaitanya K and Laurent Thomas and Bengio Yoshua and Bresson Xavier. Benchmarking Graph Neural Networks. arXiv preprint arXiv:2003.00982, 2020

[13] M. Bronstein and Joan Bruna and Y. LeCun and Arthur Szlam and P. Vandergheynst. Geometric Deep Learning: Going beyond Euclidean data. IEEE Signal Processing Magazine, 2017

[14] Yimeng Min and Frederik Wenkel and Guy Wolf. Scattering GCN: Overcoming Oversmoothness in Graph Convolutional Networks. In NeurIPS 2020

[15] F. Gama and J. Bruna and A. Ribeiro. Stability Properties of Graph Neural Networks. In IEEE Transactions on Signal Processing, vol. 68, pp. 5680-5695, 2020, doi: 10.1109/TSP.2020.3026980

[16] Alvaro Sanchez-Gonzalez and Jonathan Godwin and Tobias Pfaff and Rex Ying and Jure Leskovec and Peter W. Battaglia. Learning to Simulate Complex Physics with Graph Networks. In ICML, 2020

[17] Bingbing Xu and Huawei Shen and Qi Cao and Yunqi Qiu and Xueqi Cheng. Graph Wavelet Neural Network. In ICLR, 2019

[18] Filipe de Avila Belbute-Peres and Thomas D. Economon and J. Zico Kolter. Combining Differentiable PDE Solvers and Graph Neural Networks for Fluid Flow Prediction. In ICML, 2020

[19] D Chenand L Jacob and J Mairal. Convolutional Kernel Networks for Graph-Structured Data. In ICML, 2020

[20] Pierre Yser and Christophe Bailly. High-Order Variational Multiscale Model in Finite Elements Applied to the LEISA-2 Configuration. In. AIAA JOURNAL Vol. 56, No. 12, December, 2018

[21] Jiong Zhu, Yujun Yan, Lingxiao Zhao, Mark Heimann, Leman Akoglu, Danai Koutra. Beyond Homophily in Graph Neural Networks: Current Limitations and Effective Designs. In Neurips, 2020