Internship Research Project - Master or Engineering degree

Using the Adjoint Method to boost the generalization of Deep Learning Models for Fluid Mechanics

Key words : Adjoint Method, Partial Differential Equations, Navier Stokes Equations, Computational Fluid Dynamics, Graph Neural Networks.

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

1 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 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

Supervision :

1. **Extrality** : Thibaut Munzer, Lead Deep Learning Engineer.

Spin off : possibility to pursue with a PhD.

Internship Outcomes : patents and / or publications in conferences.

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

2 Extrality R&D

Extrality frees industrial design and enables manufacturers in aerospace, transports and energy to drastically reduce their time-to-market.

Our AI-powered simulations platform allows engineers to assess aerodynamics, fluids and thermics of a product in just a few seconds while keeping industry-critical physical accuracy (four pending patents). We want to empower engineers to focus on what really matters, i.e. building disruptive products, instead of wasting time on long and tedious computations.

Our vision : go fast, go wild, go safe.

We are a team of 15 international level experts combining ML and Physics knowledge, and are passionate about mastering tomorrow's complex industrial and environmental challenges and empowering people through the next generation of AI.

Our Values :

- **Transparency**: We want everyone to feel aware of all the company's information and we promote feedbacks between each others
- **Excellence**: We think that every details matters and that continuous learning is the key to success
- **Resilience**: Whatever the obstacles we face, we overcome them
- **Curiosity**: We allow time for everyone to explore new ideas and keep up with the work of others

Why join Extrality ?

- To be part of a fast-learning environment and an entrepreneurial journey
- To have a wide variety of missions and a lot of autonomy
- To work with passionate people who will share their knowledge and help you develop and grow

Extrality guarantees equal opportunity for all during the recruitment process, without any distinction of gender, ethnicity, religion, sexual orientation, social status, disability or age.

General information

- **Company**: Extrality
- **Starting date**: March- April for 6 months
- **Location**: Agoranov, 96bis Bd Raspail, 75006, Paris
- **Advantages**: 50% on Navigo subscription, lunch tickets with Swile and competitive salary
- **Contact**: jobs@extrality.ai with [**ML Internship**] in the subject

3 Context of internship

The conception of industrial products like cars, planes, rockets, wind turbines, boats, etc, required to be tested in a virtual world instead of building a costly and dangerous prototype. These processes 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 the huge quantity of data extracted from numerical simulation solutions is 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 (DL) is particularly interesting thanks to its universal approximation properties; capable of approximating a wide range of continuous functions, which makes it a relevant candidate to tackle physics 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 DNNs.

3.1 Purpose of the internship

The goal of the internship is to study how the gradient computed with the adjoint method can be used to boost the generalization capabilities of deep learning models. The adjoint method allows computing the derivative of some target quantity w.r.t. every single point coordinate of the input shape when the quantity of interest is governed by a PDE. At a very high level, the adjoint method consists in solving the dual problem of the linearized PDE to compute the gradient in a very efficient manner (the number of computations is independent of the number of parameters for which the gradient is computed). It is used in the CFD industry to speed up shape optimization among others.

The goal of the internship is to study how these gradients can be used to train a deep neural network. We believe that by training a network to not only predict the correct fluid dynamics but also their derivative, it is possible to greatly reduce the number of simulations needed to achieve industry-grade results. There is however a lot of open questions on how to best achieve that objective.

The first part of the internship will consist in proposing and evaluating an approach on a 2D use case. The network architecture can be a CNN or Graph Neural Network (GNN) depending on the intern preferences. A dataset of fluid simulation and their adjoint solution will be given to the intern to conduct this study. Based on the results of this first part and the time to get them, applying the method to an industrial use (3D) case might be pursued.

During the internship you will

- Study related state-of-the-art works
- Make an exhaustive ablation study including qualitative and quantitative assessments as well as theoretical analysis
- Define appropriate metrics to evaluate your models
- Be encouraged to make regular scientific presentations for ML and Physics team and / or scientific vulgarization for Extrality group
- Participate to our weekly paper presentations, weekly coffee paper discussions and monthly seminar with external speakers.
- Make a patent and / or publish your work in a conference

References

[1] THUEREY, Nils, WEIßENOW, Konstantin, PRANTL, Lukas, et al. Deep learning methods for Reynolds-averaged Navier–Stokes simulations of airfoil flows. AIAA Journal, 2020, vol. 58, no 1, p. 25-36.

[2] SANCHEZ-GONZALEZ, Alvaro, GODWIN, Jonathan, PFAFF, Tobias, et al. Learning to simulate complex physics with graph networks. In : International Conference on Machine Learning. PMLR, 2020. p. 8459-8468.

[3] JAMESON, Antony. Aerodynamic shape optimization using the adjoint method. Lectures at the Von Karman Institute, Brussels, 2003.

[4] BRADLEY, Andrew M. PDE-constrained optimization and the adjoint method. Technical Report. Stanford University. https://cs. stanford. edu/ ambrad/adjoint$_{t}utorial.pdf$, 2013.