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PROGRAMME DE RECHERCHE
NUMÉRIQUE POUR L'EXASCALE

Uncertainty Quantification for the closure modeling of the turbulent Reynolds stress tensor

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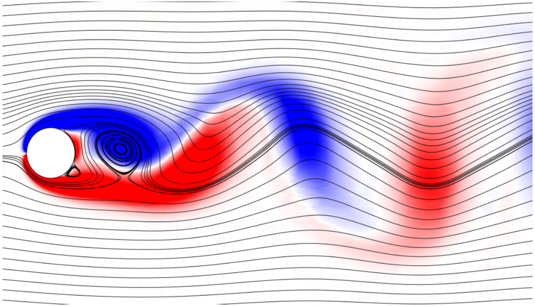
Presentation

- Nassouradine Mahamat is a PhD Student in **CEA Saclay** under the supervision of **Clément Gauchy** (CEA Saclay), and is directed by Prof. **Sébastien Da Veiga** at ENSAI CREST.
- Thesis subject : **Uncertainty quantification for the closure modeling of the turbulent Reynolds stress tensor**.
- The PhD program is a part of the **ANR project Exa-MA** (Methods and Algorithms for Exascale) under the France 2030 initiative.
- **Background** : I obtained a Master's degree in Applied Mathematics from the **University of Reims Champagne-Ardenne**, specializing in scientific computing.
- My M2 internship was part of the subject of this PhD program as preliminary work, where I worked on the theme of the **prediction of physical fields under linear constraints** at CEA Saclay

Context



Incompressible Navier-Stokes equations:

$$\frac{\partial u_i}{\partial x_i} = 0$$
$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{R_e}\frac{\partial^2 u_i}{\partial x_i^2} \quad (1)$$

Averaged Navier-Stokes equations (RANS) :

$$\frac{\partial \langle u_i \rangle}{\partial x_i} = 0$$
$$\langle u_i \rangle \frac{\partial \langle u_j \rangle}{\partial x_j} = -\frac{\partial \langle p \rangle}{\partial x_i} + \frac{1}{R_e}\frac{\partial^2 \langle u_i \rangle}{\partial x_i^2} - \frac{\partial \langle \mathbf{u_i'u_j'} \rangle}{\partial x_j} \quad (2)$$

The **Reynolds stress tensor** (RST) : $\tau_{ij} = -\langle u_i' u_j' \rangle$ is determined via turbulence closure modeling and is critical for solving RANS equations.

Goals

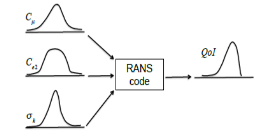
In general : Develop an uncertainty quantification framework for the RST modeling

Current objectives : Uncertainty propagation

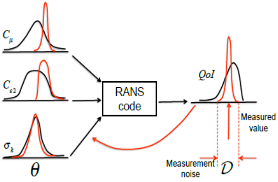
- Construction of a surrogate model for the Reynolds stress anisotropy tensor **b** by Gaussian process regression based on the Pope's model :

$$\mathbf{b} = \sum_{n=1}^{10} g^{(n)}(\lambda_1^*, \ldots, \lambda_5^*)\mathbf{T}^{*(n)} \tag{3}$$

- Develop a mathematical framework to statistically describe the RST field, by defining risk statistics. In another way, how can the concept of a quantile, defined for a real random variable as an order statistic, be applied to a set of n high-dimensional fields $(\mathbf{b}_1, \ldots, \mathbf{b}_n)$?



(a) Uncertainty propagation (forward propagation)



(b) Statistical inference (backward analysis)

To model the anisotropic RST field **b**, we need to model the strain rate tensor field **S** with the physical constraint $\mathbf{Tr}(\mathbf{S}) = 0$. This lead us to solve the following problem.

Problem statement

In this work, we are considering the multi-output regression task of finding $\mathbf{f} = [\mathbf{f}_1^T, \dots, \mathbf{f}_Q^T]^T : \mathcal{X} \to \mathbb{R}^P$ such that:

$$\begin{aligned} \mathbf{y} &= \mathbf{f}(\mathbf{x}), \quad \mathbf{y} \text{ is a high dimensional vector, i.e } P \approx 10^4 \\ \mathcal{F}[\mathbf{f}(\mathbf{x})] &= \sum_{j=1}^{Q} \alpha^j \mathbf{f}^j(\mathbf{x}) = \mathbf{c}(\mathbf{x}) \end{aligned} \tag{4}$$

- Gaussian process regression, originally introduced in geostatistics as kriging, is widely used in metamodeling for its probabilistic framework, which captures prediction uncertainty.
- An extension of Gaussian processes (GPR) to multivariate outputs, known as Multi-output Gaussian Process[1], has been developed in the literature, with applications in time series and robotics. However, its $O(N^3 + P^3)$ complexity makes optimization expensive when N (data size) or P is large.
- We must reduce the output dimension P to avoid this complexity.

[1] Alvarez, Mauricio A., Lorenzo Rosasco, and Neil D. Lawrence. Kernels for vector-valued functions: A review. *Foundations and Trends® in Machine Learning* 4.3 (2012): 195-266

Conclusion

- If you are interested in estimating quantiles of simulated physical fields using HPC, feel free to share with us your interest.
- **Thanks! Any questions ?**