Novel Resampling Strategies to Improve Surrogate Model in an Uncertainty Quantification Framework

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Abstract:

CFD codes have reached a sufficient maturity to represent physical phenomena, and complex flow simulation on high-resolution grid is becoming possible with continuous developments in numerical methods and in High Performance Computing (HPC). Still, deterministic simulations only provide limited knowledge on a system as uncertainties in the numerical model and its inputs translate into uncertainties in the outputs.

In fact, the diversity of uncertainties on the initial conditions, as well as on the model parameters (input data geometry, simplification of the model physics, etc.) limits the validity: the quantity of interest (QoI) can be easily shadowed by the conjugation of all types of uncertainties. This assessment explains why Uncertainty Quantification (UQ) is now becoming a mandatory step in application-oriented modeling for operational and industrial purposes. It provides knowledge on the level of uncertainty in the numerical simulation results, as well as, Sensitivity Analysis (SA) which aims at describing the respective influences of some parameters on the QoI [4]. This is why the inclusion of Uncertainty Quantification in a design optimization cycle allows manufacturers to design faster and obtain better, cheaper and more robust (i.e. less uncertainty sensitive) products.

Classical UQ methods based on random *Monte-Carlo* approaches implies a large number of CFD simulations, which quickly goes beyond the limits of available computational ressources especially when it comes to large dimension problem. However, the cost of UQ study can be significantly reduced when the CFD code is replaced by a surrogate model which is formulated in a reduced space and which is fast to evaluate for any set of uncertain variables.

The surrogate model can consist of a polynomial interpolation, a polynomial chaos expansion or, in case of a functional output, a successful approach —which is considered here— consists in combining Gaussian Process with POD [5][2]. In any case, the number of CFD simulations that are required for the formulation of the surrogate model is determinant.

The accuracy of an uncertainty quantification being directly correlated to the quality of the surrogate, this work aims at improving its construction by resampling the space of parameters using novel approaches. Starting from a low discrepancy sequence [3] and from the work of Scheidt *et al.* [6], three methods have been assessed :

- Mean Square Error (MSE),
  One of the main advantages of Gaussian processes is to give an insight into the variance of the solution. The first method consists in using this error (MSE) and weight it with the modes of the POD. The maximal error point is selected for refinement.
- Leave-One-Out Cross Validation (LOOCV) and MSE,
  A LOOCV is performed on the POD. This gives the point where the model is the more

sensitive if deleted. The strategy is thus to add a new point around it. To do so, a hypercube is created and within it, a global optimization over the MSE is conduced giving the new point.

- LOOCV-Sobol',
  Using the same steps as with the LOOCV-MSE method, the hypercube around the point is here modified using prior information about Sobol' indices. It requires that indices are closed from converged in order not to bias results. The bias can be intentional depending on the insight we have about the case.

This work is part of an ongoing project which aims at performing UQ on a LES case. It consists in perturbing the turbulence intensity T_u and the inflow angle α on a turbine cascade configuration [1]. Preliminary results exhibit a major contribution of T_u over α. Still, the model has been computed using 24 simulations leading to an estimated quality $Q_2 \sim 0.7$. Refining the space of parameters would enhance the statistical analysis and allows to better understand the physical phenomena.

References

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Short biography – After a master degree in Aeronautics and Aerospace at IPSA, I went to ISAE-SUPAERO to conduce an advance master in Aeronautics and Aerospace propulsion where I discover the Computational Fluid Dynamics field. This leads me to the CERFACS where I had the opportunity to perform an internship on Uncertainty Quantification applied to blade design in a Large Eddy Simulation context. Now I have the chance to continue with a PhD thesis on UQ with the objective to reduce the number of simulation needed.