



# Uncertainty analysis as an ally for deep-learning-based hybridization of simulation codes

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## Abstract:

In numerical simulations and computational physics, many challenges stem from a trade-off between the accuracy of computational codes and their cost-efficiency. Indeed, a numerical simulation has to model physics as finely as possible to be accurate and reliable. Nonetheless, in that case, the code execution can be computationally intensive and sometimes even not affordable. Finding the right level of accuracy to reliably simulate a phenomenon and the right amount of simplifications to make it workable is a complex task. In this talk, we contribute to this effort for a stationary hypersonic reentry code based on Euler equations coupled with chemical equilibrium. We accelerate this code using hybridization between the fluid dynamic solver and a neural network surrogate model trained to approximate the solution of the chemical equilibrium solver. By doing so, we emphasize how valuable uncertainty quantification can be in that context. More specifically, we adapt and use sensitivity analysis to optimize the neural networks' hyperparameters, which yields cost-effective and accurate surrogate models. Then, we use uncertainty quantification to provide guarantees for the hybrid code.

## 1 Deep learning-based hybridization for accelerating the coupling between hypersonic reentry and chemical reactions

We consider the stationary simulation of the hypersonic reentry of an object coupled with chemical reactions. The solver used for the fluid dynamics is not expensive when executed alone. However, the solver used to simulate the chemical reactions needs to be called at each time step and at each mesh cell to simulate chemical reactions, which dramatically increases the computation time.

In this work, we tackle this challenge by constructing a hybrid numerical simulation based on the coupling of the fluid dynamic with a neural network simulating chemical reactions. This approach is motivated by several considerations. First, the solver used to simulate the chemical reactions can be executed as a standalone application, so we can build an extensive training database and train the model in an offline mode. Second, the complexity of neural networks is independent of the size of the database, so we can leverage this large database without affecting its execution speed. Moreover, it is linear with the input/output dimension, so we can potentially consider more chemical reactions. Finally, their implementation boils down to matrix-vector products, which enables to easily and efficiently vectorize the simulation of chemical reactions.

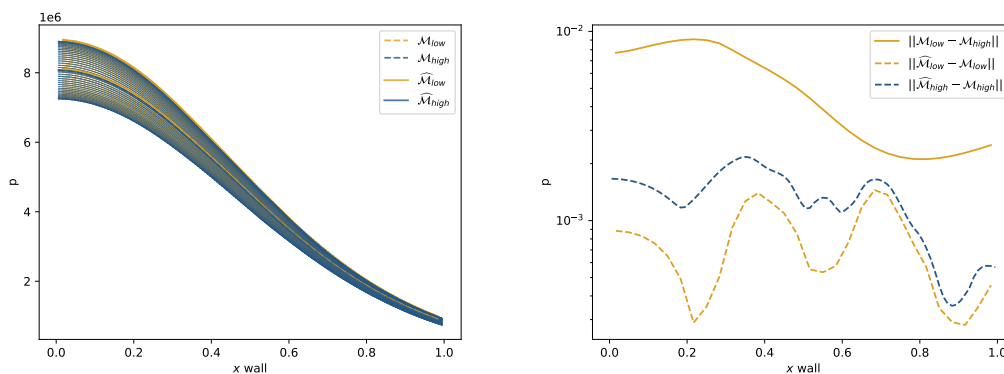
We first design a neural network with a random hyperparameter search and use it to construct the hybrid code,  $\widehat{\mathcal{M}}$ . We compare its performances and the quality of its prediction with those of the original code  $\mathcal{M}$ . We obtain an error of  $6.06 \times 10^{-7}$  in the pressure profile at the boundary of the object with an acceleration factor of 8.

## 2 Goal oriented sensitivity analysis for cost effective neural nets.

We then focus on the design of the neural network that we use for the hybrid code. We apply an uncertainty analysis approach, inspired from [2] to the context of hyperparameter optimization. We adapt Hilbert Schmidt Independence Criterion [1] in its goal-oriented version to hyperparameters space. This is not straightforward because hyperparameters can be categorical, continuous, discrete, boolean (e.g. activation function vs learning rate), they can interact (e.g. batch size and optimizer) or may not be always involved in the training (e.g. different optimizers parameters), which makes their direct comparison non-trivial. We alleviate those concerns and design and use HO methodologies that make use of the knowledge stemming from this sensitivity analysis. Finally, we obtain a neural network which, once embedded into the code  $\widehat{\mathcal{M}}$ , keeps the same accuracy but unlocks an acceleration factor of 18.7. These results are promising but have only been obtained on one instance of the considered test case. To be able to use the hybrid code reliably, we would like to design accuracy guarantees. For that purpose, once again, uncertainty analysis can be helpful.

## 3 Uncertainty quantification to obtain guarantees

We call the error of  $\widehat{\mathcal{M}}$  the hybrid error. We also consider other sources of errors that are classical in numerical simulations, namely the discretization error and the parameters' uncertainty error. To assess if the hybrid error is acceptable, we perform a convergence study: we compare the results obtained on a coarse (low) and a fine (high) mesh for  $\widehat{\mathcal{M}}$  and  $\mathcal{M}$ ; and an uncertainty propagation: we consider the upstream fluid velocity as uncertain (since it is classically considered the most influential source of uncertainty). Let us denote the low-resolution version of the original code  $\mathcal{M}$  by  $\mathcal{M}_{low}$ , and so on for



(a) Pressure profile at the boundary of the object. (b) Mean hybrid error vs mean discretization error.

the high resolution and other  $\mathcal{M}$  and  $\widehat{\mathcal{M}}$  codes. Figure 1a shows that the hybrid error is far lower than the fluctuations relative to the parameters' uncertainties. Figure 1b shows that the hybrid error is lower than the spatial discretization (mesh) error. Therefore, we can safely use the hybrid code to perform reliable studies.

### References

- [1] Arthur Gretton, Olivier Bousquet, Alex Smola, and Bernhard Schölkopf. Measuring statistical dependence with hilbert-schmidt norms. In *Proceedings of the 16th International Conference on Algorithmic Learning Theory*, ALT'05, page 63–77, Berlin, Heidelberg, 2005. Springer-Verlag.
- [2] Adrien Spagnol, Rodolphe Le Riche, and Sébastien Da Veiga. Global sensitivity analysis for optimization with variable selection. *SIAM/ASA J. Uncertain. Quantification*, 7:417–443, 2018.

**Short biography** – I graduated from Telecom Paris, with an MSc in Statistics from Imperial College London, in 2018. Then I started a PhD at CESTA, CEA-DAM; Inria Saclay; and CMAP, Ecole Polytechnique on the application of Deep Learning in a HPC numerical simulation context. I study the acceleration of simulation codes with the help of artificial neural networks and uncertainty analysis.