Uncertainty Quantification for Scientific Machine Learning Models

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Start Upon agreement
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Problem setting

Numerical simulations are indispensable for numerous applications, as they allow scientists and engineers to investigate *in silico* phenomena that would otherwise be too difficult or expensive to observe and study. At the same time, high-fidelity simulations can be time- and resource-demanding, often requiring significant computing resources and long simulation times. This computational burden becomes especially problematic considering repeated analysis tasks, such as optimization, uncertainty quantification, or sensitivity analysis.

To render tasks that necessitate repetitive computations feasible, practitioners often resort to *surrogate models* (also called *metamodels* or *emulators*) that approximate the input-output map of a costly simulator [1]. One common approach is to construct surrogate models from available datasets using machine learning (ML), for example, by means of regression, dimension reduction, or their combination. More recently, *scientific ML (SciML)* methods that combine ML with physics-based modeling principles [2] are getting traction in the context of surrogate modeling.

However, most data-driven surrogate models based on either pure ML or SciML produce point estimates that lack information regarding the uncertainty in their predictions. For model-based estimates that may affect safety, cost, or scientific conclusions, information about predictive uncertainty is often as important as the prediction itself. This is particularly relevant for data-scarce applications in physics and engineering.

Thesis' goal

This thesis will develop methods for attaching reliable predictive uncertainty intervals to SciML surrogate models using *conformal prediction (CP)* [3]. It will combine algorithmic development, careful empirical evaluation, and domain-aware design to produce predictive UQ tools that are both statistically principled and usable in data-scarce, physics-driven workflows. Exemplary objectives to be pursued include (but are not limited to):

- Implementation and comparison of different CP variants for representative surrogate models.
- Design of non-conformity measures that incorporate physics knowledge or model structure [4].
- Uncertainty-aware surrogate modeling for dynamical physical systems [5].

The work will combine theoretical justification with numerical experiments. Key evaluation criteria will be empirical coverage (versus target coverage), predictive interval efficiency, robustness under data scarcity, computational cost, and ease of integration with existing SciML workflows. Numerical experiments shall include calibration size sensitivity studies and comparisons to baseline UQ approaches (for example, predictive intervals of Gaussian process models).

References

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*Possibility for co-supervision with Dr. Stéphane Lanteri, head of the ATLANTIS team at Inria Centre at Université Côte d'Azur. In that case, electromagnetic field applications will be considered. A short-term stay at Inria will also be organized.