Physics-informed, boundary-constrained Gaussian processes with applications in fluid dynamics

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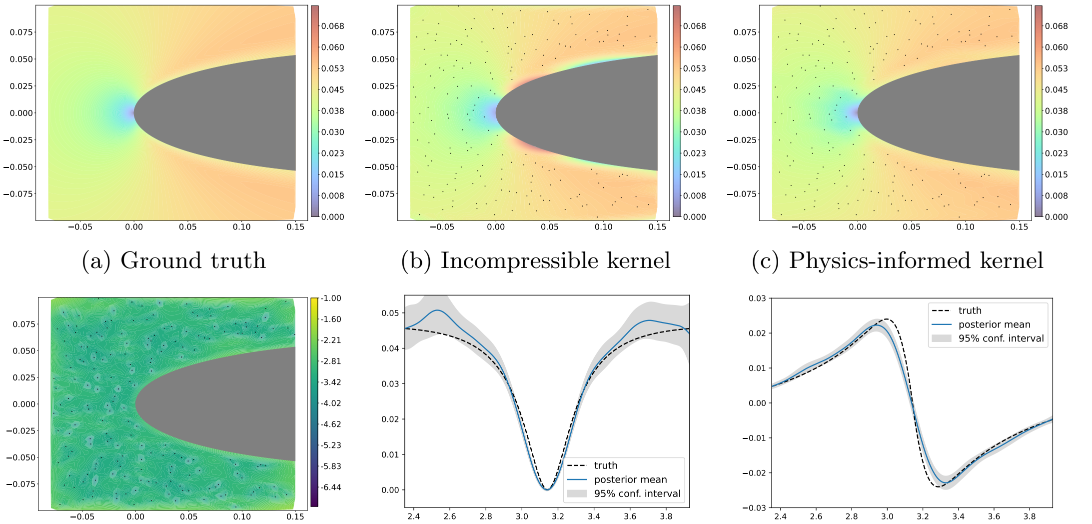
Abstract

In this communication we present a framework for surrogate modelling of incompressible fluid flows using Gaussian processes (GP) constrained by physical conditions and including uncertainty quantification (UQ). We develop a general method to continuously enforce a prescribed GP on an arbitrary compact subset of its domain. Other methods that explore boundary conditions on GPs are based on defining particular structures of the covariance kernels or are not necessarily adapted to consider derivatives of the GP. The proposed strategy uses a spectral expansion of the prescribed GP on the compact set, which in practice corresponds to the boundary of an aerodynamic profile (*e.g.* cylinder, NACA airfoil), to enforce boundary conditions. This enables us to consider observations of derivatives of the GP directly while satisfying other physical laws simultaneously. This framework can be thus flexibly merged within data assimilation schemes based on GP regression for the reconstruction of fluid flows.

Consider a two-dimensional incompressible flow with velocity field $\boldsymbol{u}$ over the computational domain Ω. This field must satisfy scalar boundary conditions $\mathcal{B}(\boldsymbol{u}) = 0$ over a compact set $\Gamma \subset \Omega$, where $\mathcal{B}$ is a scalar-valued linear operator on $\boldsymbol{u}$. In this setting the velocity field can be explained through a scalar stream function ψ such that $\boldsymbol{u} = \mathbf{curl}\,\psi = (-\partial_{x_2}\psi, \partial_{x_1}\psi)^\mathsf{T}$. Our strategy consist in modelling the stream function as a GP prior Z, so that the velocity field can be modelled as $\mathbf{curl}\,Z$, verifying thus the divergence-free condition (from incompressibility) $\partial_{x_1}u_1 + \partial_{x_2}u_2 = 0$ everywhere in Ω. Furthermore, a power-law structure for the energy decay of velocity increments can be accounted for in the definition of the covariance kernel $\boldsymbol{K}$ of $\mathbf{curl}\,Z$, as illustrated in [2, 3]. Lastly, boundary information on the profile delimited by Γ can be included by using our general spectral method [3] based on [1]. In this sense we obtain a modified version $\boldsymbol{K}_0$ of $\boldsymbol{K}$ satisfying also the homogeneous boundary condition everywhere and not only at a discrete set of observations.

Now, given a set of velocity measurements $\boldsymbol{V}(t)$ at positions $\boldsymbol{X}(t)$ (*e.g.* Lagrangian data in particle tracking velocimetry), this physics-informed GP prior can be used for reconstruction of the field as $\boldsymbol{u}^\star(\boldsymbol{x}, t) = \boldsymbol{K}_0(\boldsymbol{x}, \boldsymbol{X}(t))\boldsymbol{K}_0(\boldsymbol{X}(t), \boldsymbol{X}(t))^{-1}\boldsymbol{V}(t)$. UQ counterparts follow in a similar manner, as well as posterior estimates for the stream function ψ and vorticity $\omega = \mathbf{curl}^\mathsf{T}\boldsymbol{u}$. Main results are depicted in Figure 1. In [3], we compare the reconstructions with respect to three choices of the covariance kernel of Z: an incompressible radial basis function (RBF), a multi-scale additive RBF, and the physics-informed boundary-constrained kernel as described above. The calibration of hyperparameters is performed by cross-validation using UQ coverage indicators of the estimates.



(a) Ground truth (b) Incompressible kernel (c) Physics-informed kernel

(d) Uncertainty quantification (e) Horizontal velocity (f) Vertical velocity

Figure 1: **Reconstruction of the velocity field $\boldsymbol{u}$ of an incompressible flow around the leading edge of a NACA 0412 airfoil [3].** Ground truth field is depicted in (a), with colormap as velocity norm in m/s. In (b), the reconstruction of the field is done from 184 velocity measurements $\boldsymbol{V}$ (black dots •) using GP regression with a one-scale incompressible kernel. In (c), the kernel is further informed with the profile boundary condition (slip) and an energy decay law [3]. This last physics-informed estimate $\boldsymbol{u}^\star$ comes with the UQ counterpart depicted in (d), as the (logarithmic) total standard deviation. Notice that even if there are no discrete measurements at the airfoil boundary, the physics-informed kernel $\boldsymbol{K}_0$ used in (c) is able to capture the velocity field, as displayed in (e) and (f) for each spatial component (horizontal axis is domain of airfoil boundary Γ parameterization).

We further explore the use of this framework to define a data assimilation scheme using the numerical method on the Navier-Stokes equations for vorticity from [2]. Preliminary tests indicate that this scheme can accurately propagate the initial information through subsequent assimilation steps, incorporating Lagrangian velocity and vorticity measurements when available. Moreover, it is competitive in comparison to its pure data-driven version in scarce data regimes. We are also interested in optimal sensor placement to improve the reconstructions using UQ of the estimates.

Short biography (PhD student)

This research project is at the intersection of probabilities, data assimilation and numerical analysis of differential equations. Adrian Padilla–Segarra holds a MSc from Paris–Saclay University (track Analysis, Modelling, Simulation at Orsay and ENSTA, under a FMJH scholarship) and a BSc in Mathematics from Yachay Tech (Ecuador). The PhD project is jointly financed by ONERA and INSA Toulouse (SHOM project "Machine Learning Methods in Oceanography" no-20CP07) and is attached to the IMT. A collaboration with prof. Houman Owhadi from Caltech (Pasadena, United States) is ongoing.

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