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# Constrained reduced-order modelling of reacting flows

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**Abstract:**

Reduced-order models (ROMs), combining computational fluid dynamics simulations with dimensionality reduction techniques like Proper Orthogonal Decomposition (POD) and non-linear regression methods such as Gaussian Process Regression (GPR), provide an accurate approach for analyzing high-dimensional combustion problems. However, this approach may yield physically inconsistent results, such as negative mass fractions. While POD complicates constraint enforcement in the reduced space due to its linear nature, GPR lacks inherent physical constraints. This study develops constrained ROMs of combustion systems to ensure physical consistency while maintaining accuracy. We propose downsampling the dataset via optimal sensor placement using low-cost Singular Value Decomposition (lcSVD) [1]. This technique selects points that preserve physical information, enabling constraints in GPR. We employ parametric distribution functions with finite support, such as truncated Gaussian and beta distribution scaled to the interval $[a, b]$, to define the GP likelihood function within a variational inference framework [2]. These non-Gaussian likelihoods inherently produce GP observations that satisfy the constraints. The frameworks are evaluated in two test cases to predict unexplored thermo-chemical states. The first involves one-dimensional laminar $NH_3/H_2$ flames with variations in equivalence ratio, $H_2$ molar fraction, and inlet temperature. The second examines three-dimensional $CH_4/H_2$ simulation samples with detailed chemistry from a semi-industrial furnace, varying air injector diameter, fuel composition (pure methane to pure hydrogen), and equivalence ratio. Results show that the Beta likelihood bounds predictions between 0 and 1 by design, while the truncated Gaussian improves robustness by reducing outliers' impact and improving reliability in sparse or noisy regions. These methods preserve the accuracy of unconstrained ROM while ensuring predictions comply with physical constraints.

**Keywords:** Reduced-order model; Gaussian Process Regression; Constrained likelihood functions; Downsampling; Combustion systems

**References:**

[1] Hetherington, A., & Clainche, S.L. "Low-cost singular value decomposition with optimal sensor placement," 2023. *ArXiv, abs/2311.09791*.

[2] Jensen, B. S., Nielsen, J. B. and Larsen, J. "Bounded Gaussian process regression," *IEEE international workshop on machine learning for signal processing (MLSP)*, pp. 1-6, IEEE, 2013.