A DATA-DRIVEN EXTERIOR CALCULUS FOR PROBABILISTIC DIGITAL TWINS

Nathaniel Trask,¹ Jonas Actor, Andy Huang,² Xiaozhe Hu,³ Houman Owhadi⁴

¹University of Pennsylvania ²Sandia National Laboratories ³Tufts University ⁴Caltech

ABSTRACT

Despite the recent flurry of work employing machine learning to develop surrogate models to accelerate scientific computation, the "black-box" underpinnings of current techniques fail to provide the verification and validation guarantees provided by modern finite element methods. In this talk we present a data-driven finite element exterior calculus for developing reduced-order models of multiphysics systems when the governing equations are either unknown or require closure. The framework employs deep learning architectures typically used for logistic classification to construct a trainable partition of unity which provides a notion of a control volume, with associated boundary operators and consequent div/grad/curl operators. This alternative to a traditional finite element mesh is fully differentiable and allows construction of a discrete de Rham complex with a corresponding Hodge theory. In this framework models may be extracted from data with the same robustness guarantees as traditional mixed finite element discretization, with deep connections to contemporary techniques in graph neural networks [1-3]. In our recent work developing digital twins, where surrogates are intended to support real time data assimilation and optimal control, we have extended the framework to support Bayesian characterization of unknown physics on the underlying adjacency matrices of the chain complex [4]. By framing the learning of fluxes via an optimal recovery problem with a computationally tractable posterior distribution, we are able to develop models with intrinsic representations of epistemic uncertainty.

REFERENCES

[1] Trask, Nathaniel, Andy Huang, and Xiaozhe Hu. "Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs." *Journal of Computational Physics* 456 (2022): 110969.

[2] Actor, J.A., Hu, X., Huang, A., Roberts, S.A. and Trask, N., 2024. Data-driven Whitney forms for structure-preserving control volume analysis. *Journal of Computational Physics*, 496, p.112520.

[3] Gruber, A., Lee, K. and Trask, N., 2024. Reversible and irreversible bracket-based dynamics for deep graph neural networks. *Advances in Neural Information Processing Systems*, *36*.

[4] Owhadi, Houman. "Computational graph completion." *Research in the Mathematical Sciences* 9.2 (2022): 27.