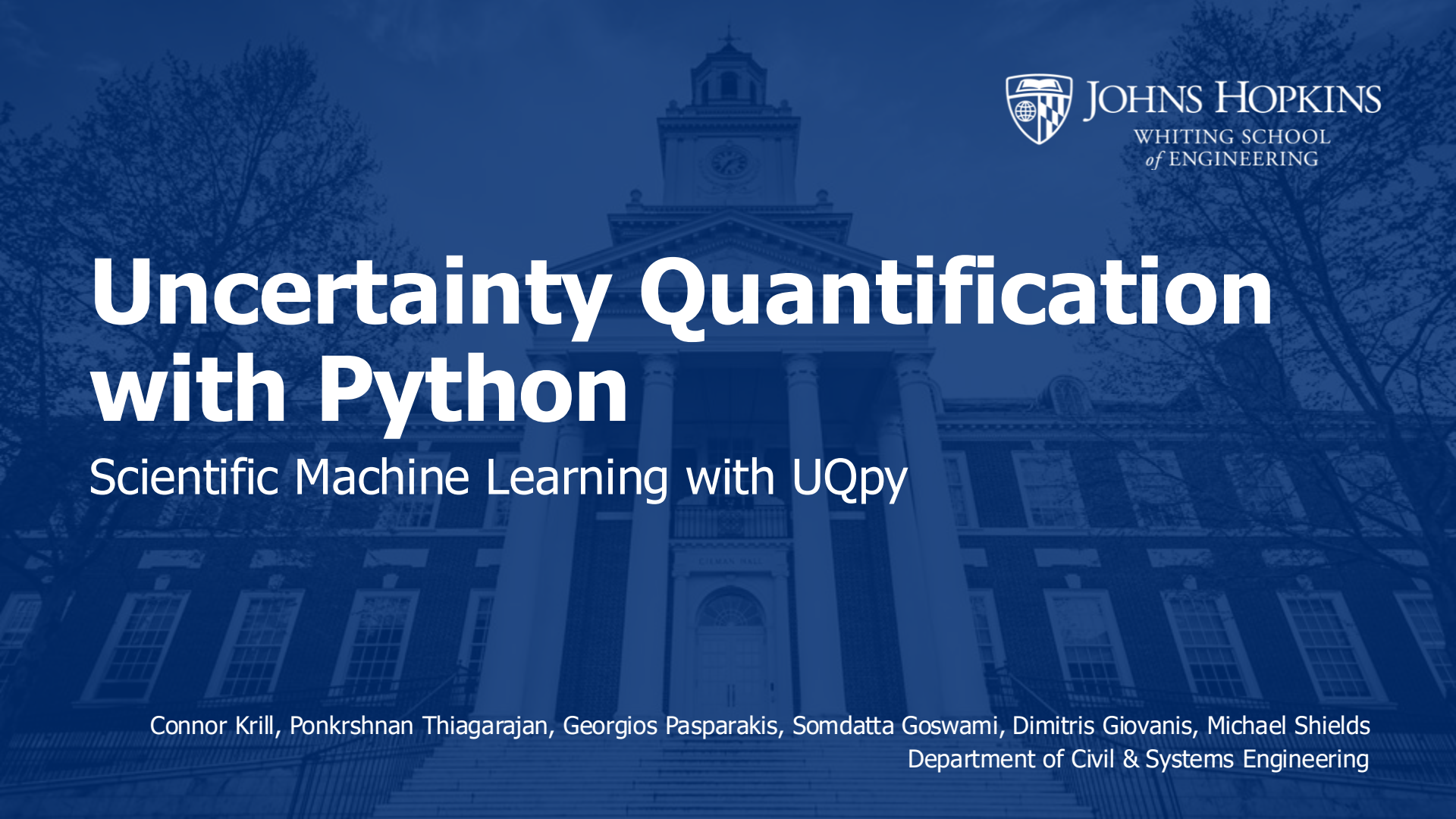


Uncertainty Quantification with Python

Scientific Machine Learning with UQpy

Connor Krill, Ponkrshnan Thiagarajan, Georgios Pasparakis, Somdatta Goswami, Dimitris Giovanis, Michael Shields
Department of Civil & Systems Engineering

Agenda

- What is UQpy?
- Software Design
- Scientific Machine Learning
  - Layers
  - Network Architecture
  - Training Methods

UQpy is a Python package where you define the **model**, and then we handle the **Uncertainty Quantification**.

UQpy Modules

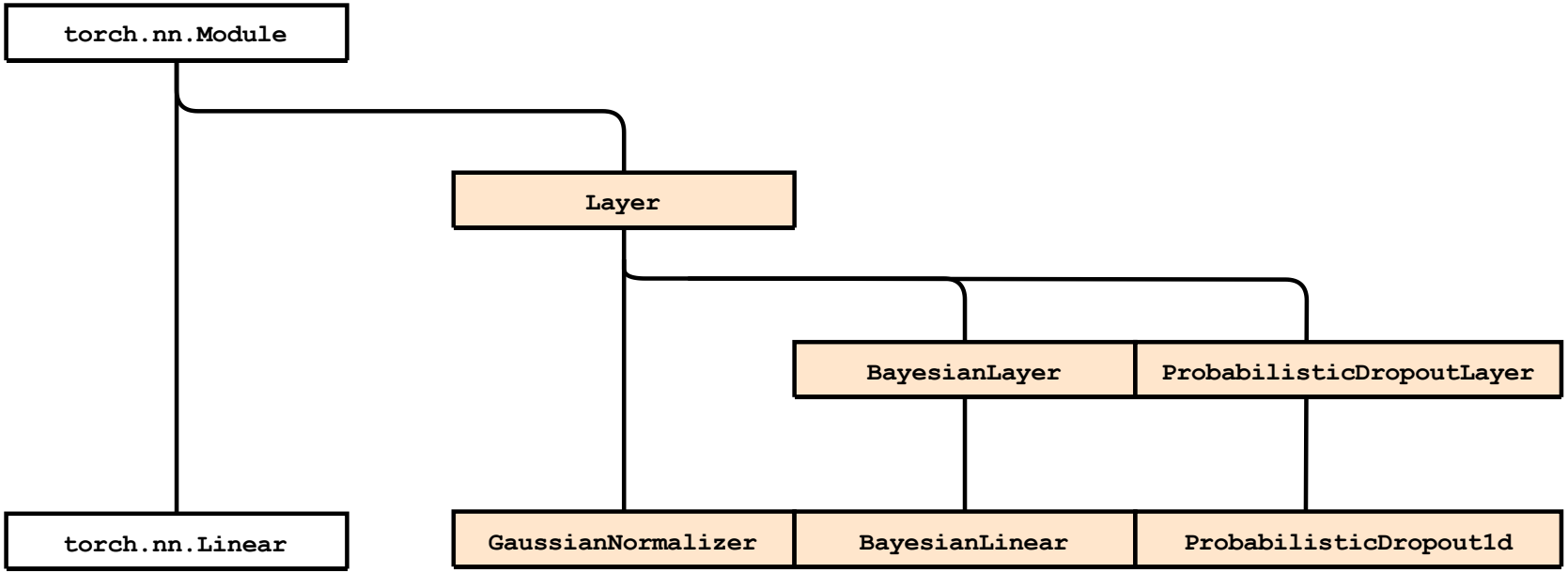
- Dimension Reduction
- Distributions
- Inference
- Reliability
- Run Model
- Sampling
- Scientific Machine Learning
- Sensitivity
- Stochastic Processes
- Surrogates
- Transformations

UQpy uses hierarchical classes to create a **modular structure** for **simple customization**.

UQpy: Scientific Machine Learning

- Incorporates UQ into PyTorch models
- Bayesian versions of Linear, Convolutions, and more!
- Architecture for Neural Operators
- Methods to train neural networks

UQpy: Scientific Machine Learning



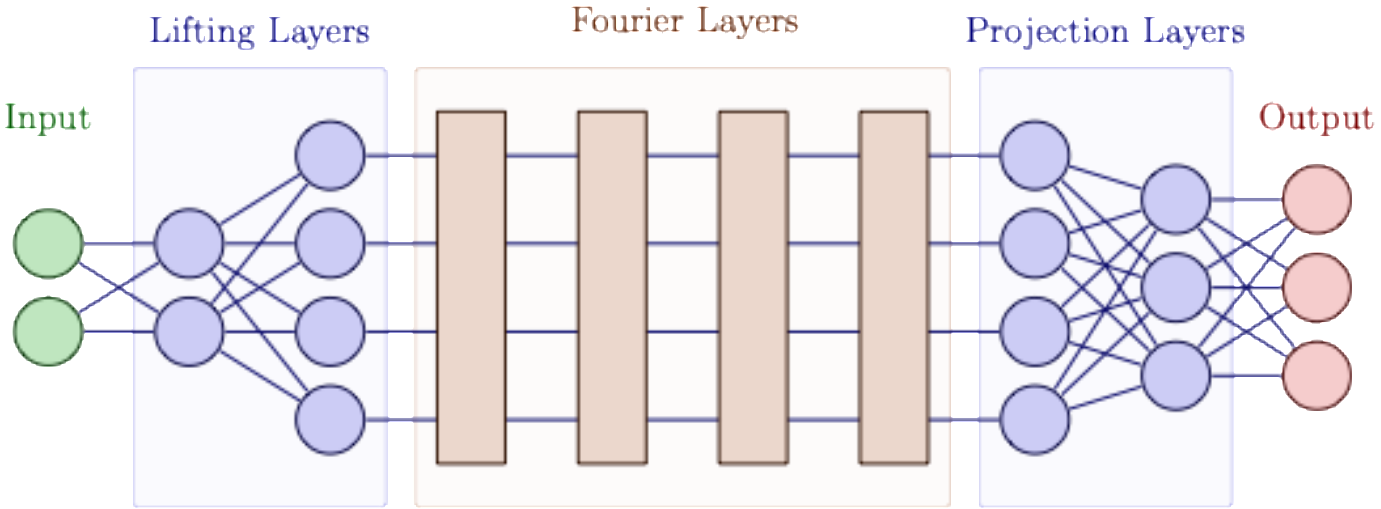
This module enables the **expansion of existing models** and the **rapid development of new research**.

SciML: Extending Existing Models

```python
deterministic = nn.Sequential(
    nn.Linear(2, 10),
    nn.ReLU(),
    nn.Linear(10, 10),
    nn.ReLU(),
    nn.Linear(10, 5),
)
```

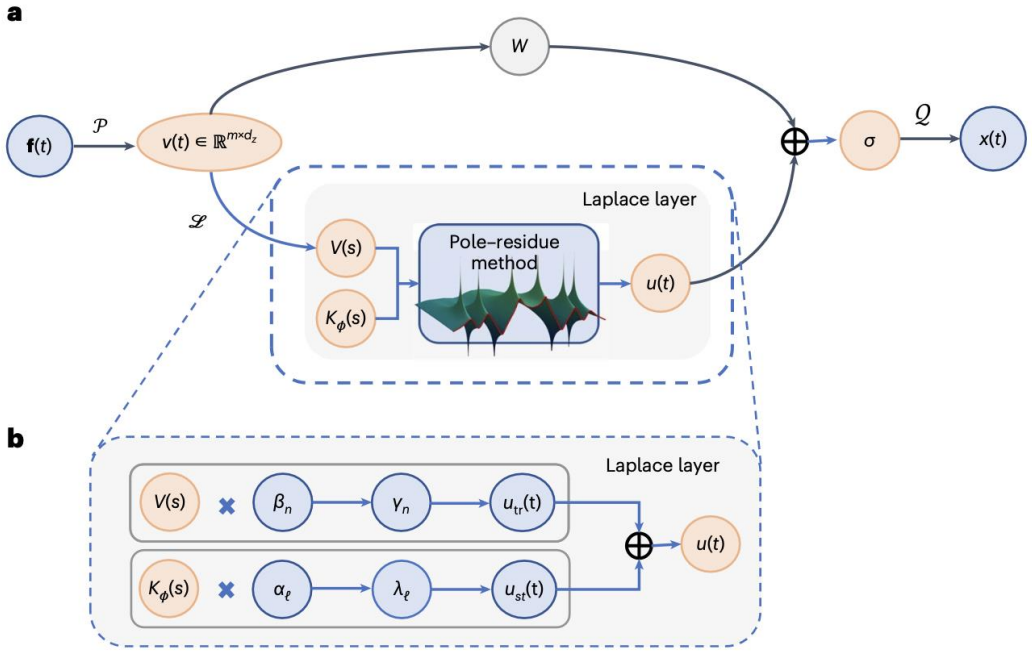
```python
bayesian = nn.Sequential(
    sml.BayesianLinear(2, 10),
    nn.ReLU(),
    nn.Linear(10, 10),
    nn.ReLU(),
    sml.BayesianLinear(10, 5),
)
```

SciML: Facilitating New Research



Architecture of a Fourier Neural Operator by Li et al. 2021

SciML: Facilitating New Research



Future Directions: Laplace Neural Operator by Cao et al. 2024

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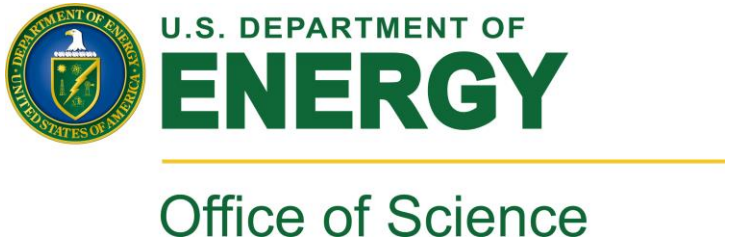
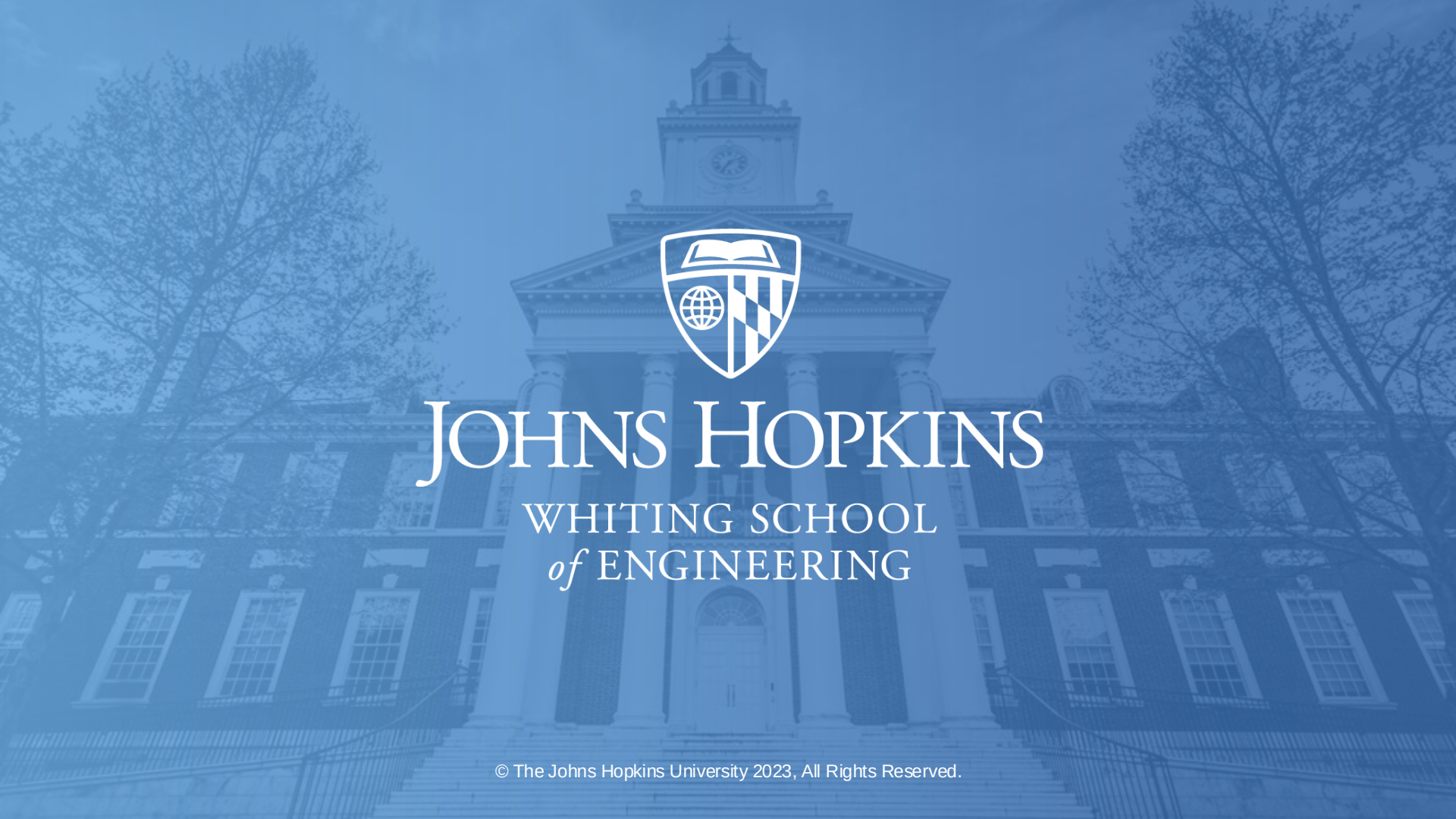


References

- Olivier, A., Giovanis, D.G., Aakash, B.S., Chauhan, M., Vandanapu, L., and Shields, M.D. (2020). *UQpy: A general purpose Python package and development environment for uncertainty quantification*. Journal of Computational Science. Volume 47, 101204. https://doi.org/10.1016/j.jocs.2020.101204
  - UQpy Documentation: https://uqpyproject.readthedocs.io/en/latest/
- Li, Z., Kovachki, N., Azizzadenesheli, K., Liu, B., Bhattacharya, K., Stuart, A., and, Anandkumar, A. (2021). *Fourier Neural Operator for Parametric Partial Differential Equations.* https://doi.org/10.48550/arXiv.2010.08895



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