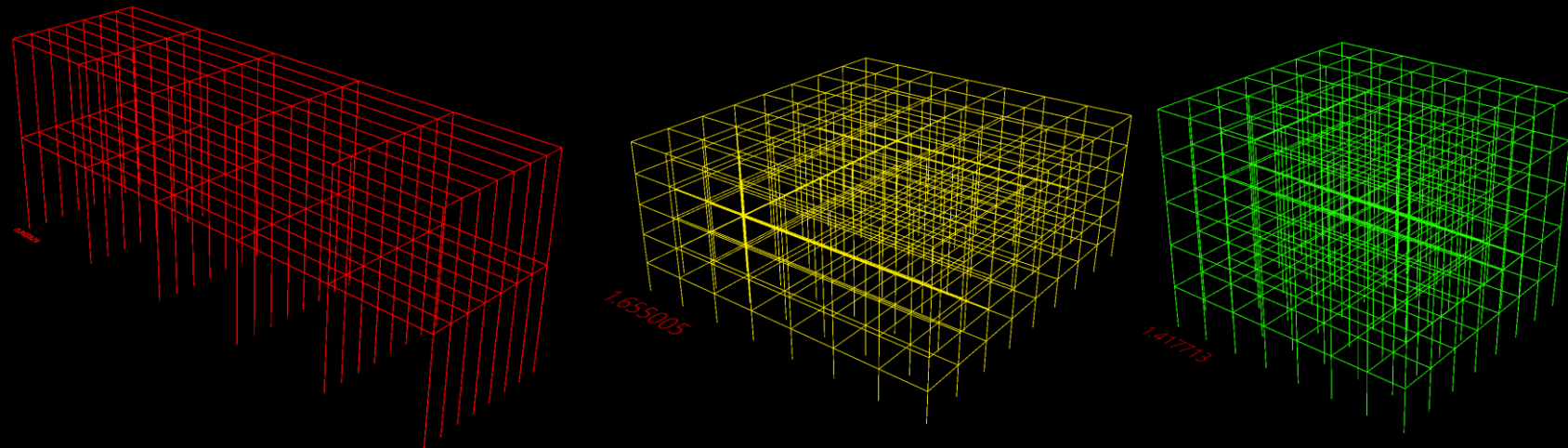


Bayesian Machine Learning for Quantifying Uncertainty in Surrogate Modelling

Archie Luxton

09:00, 14th September 2022



Background | Project Objective

Develop uncertainty-aware Neural Network-based surrogate models that can predict the modal frequencies of 3D structures and communicate the uncertainty in those predictions.

Background | Modal Analysis

- Modal analysis predicts the resonant frequencies of structures
- Modal frequencies of a structure shouldn't match frequency of:
 - Earthquakes
 - Footsteps and sway
 - Wind flutter



Mexico City earthquake, 1985



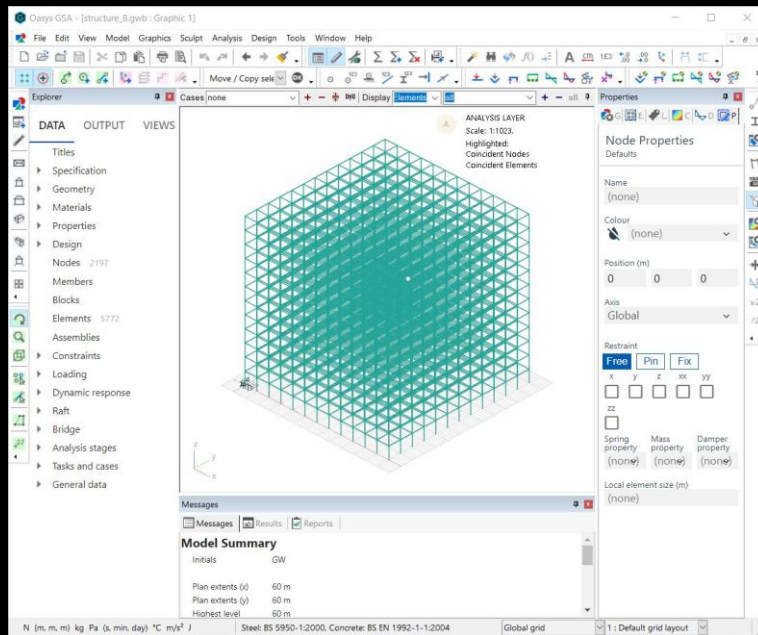
Millennium Bridge, London



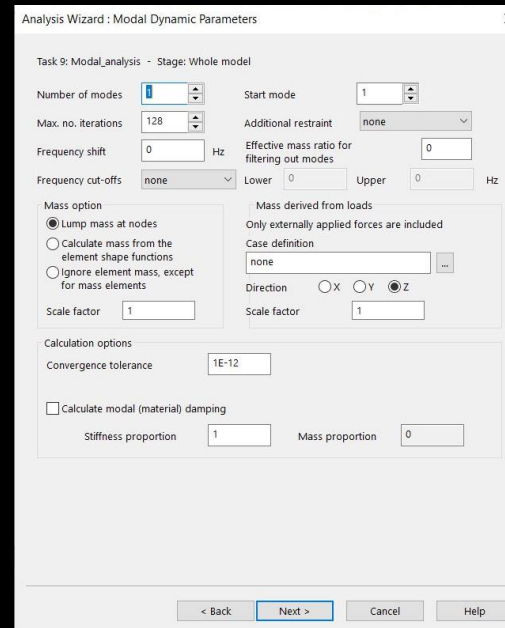
Broughton Bridge collapse, 1826

Background | Modal Analysis Using GSA

- Oasys GSA can perform modal analysis
- Calculates many modal frequencies of a structure
- Solves a generalised eigenvalue problem



Define geometry



Define simulation parameters



Wait until completion 4/17

Background | Advantages/Disadvantages of GSA Analysis

GSA Modal Analysis

Accurate

Explainable

Expensive

Complexity scales with size of structure

Platform-specific

Automation requires APIs/SDKs

Specific to one problem

Background | Surrogate Models

What?

- Lightweight models approximating physical systems/simulations

Why?

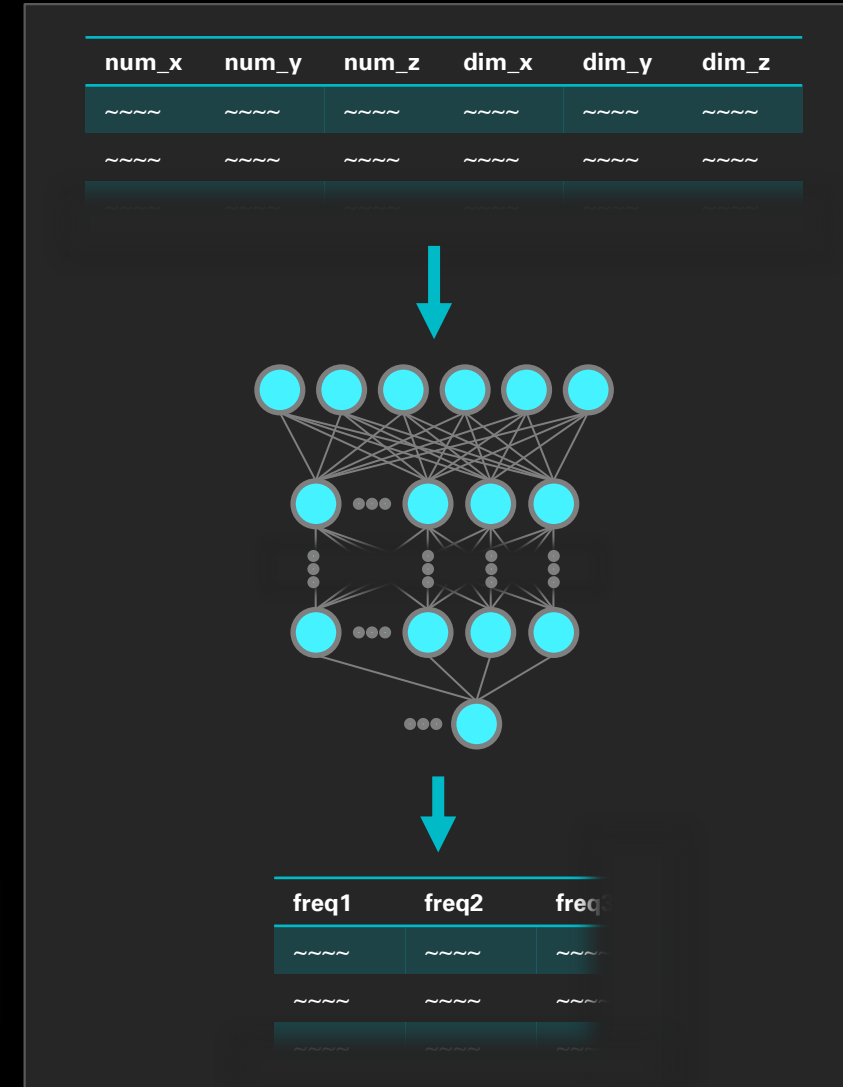
- Rapid prototyping
- Inverse problems

How?

- Neural network trained on data generated from simulations/observations



Base simulation



NN-based surrogate

Background | Surrogate vs GSA Analysis

GSA Modal Analysis	Modal Analysis via NN-based surrogate
Accurate	Is an approximation
Explainable	Challenging to explain
Expensive	Cheap predictions
Complexity scales with size of structure	Complexity constant w.r.t. size of structure
Platform-specific	Platform agnostic / portable
Automation requires APIs/SDKs	Automation very straightforward
Specific to one problem	Applicable to many problems

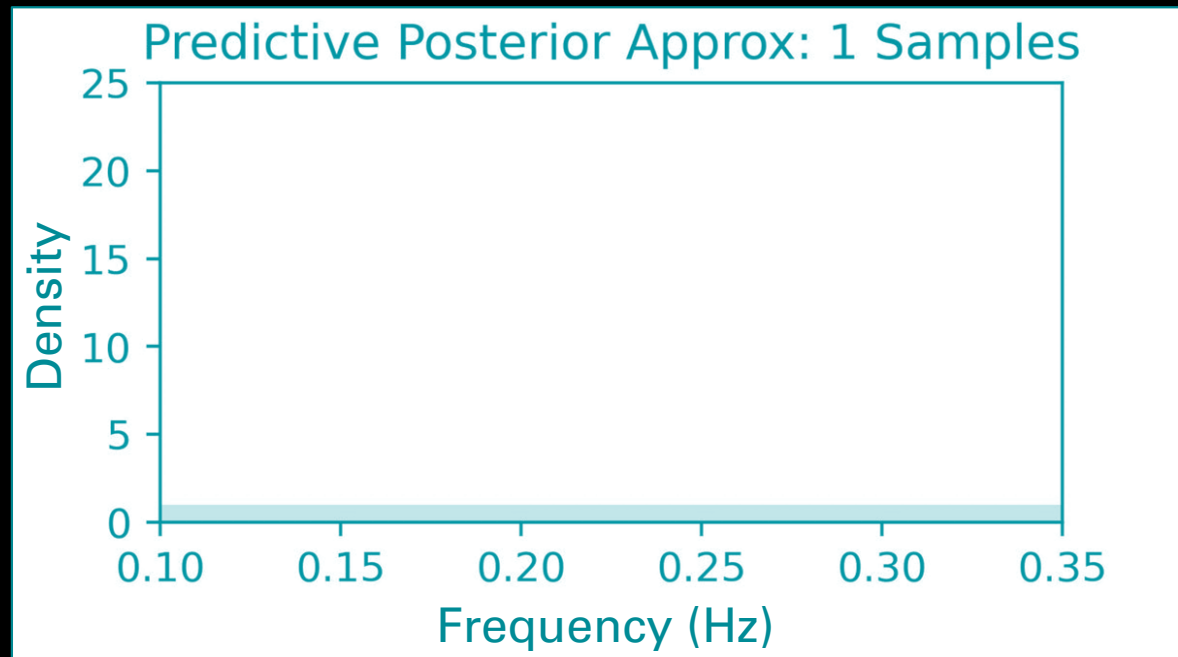
Methodology | Bayesian Neural Networks (BNNs)

→ Two Bayesian Neural Network (BNN) methods investigated:

1. MC Dropout (*Gal and Ghahramani, 2016*)
2. Stochastic Gradient Langevin Dynamics (SGLD) (*Welling et al., 2011*)

→ Both methods apply stochasticity.

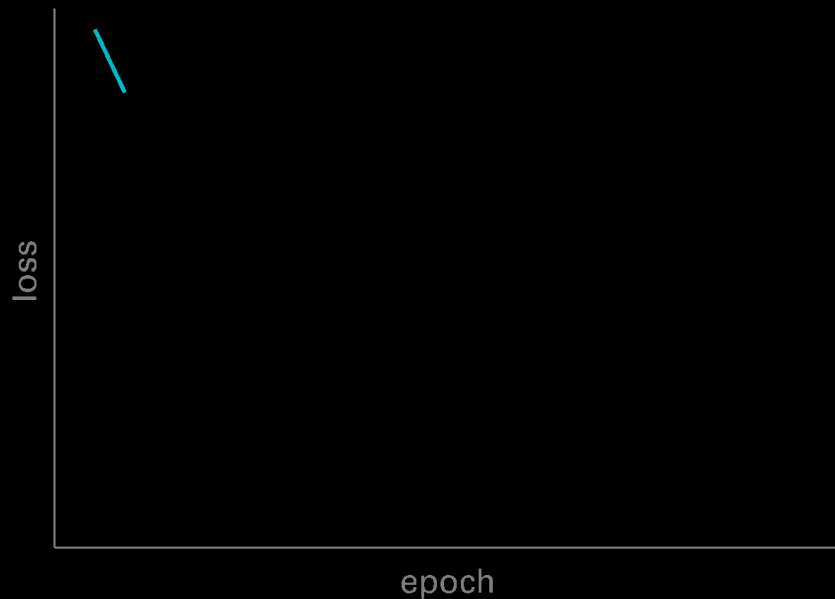
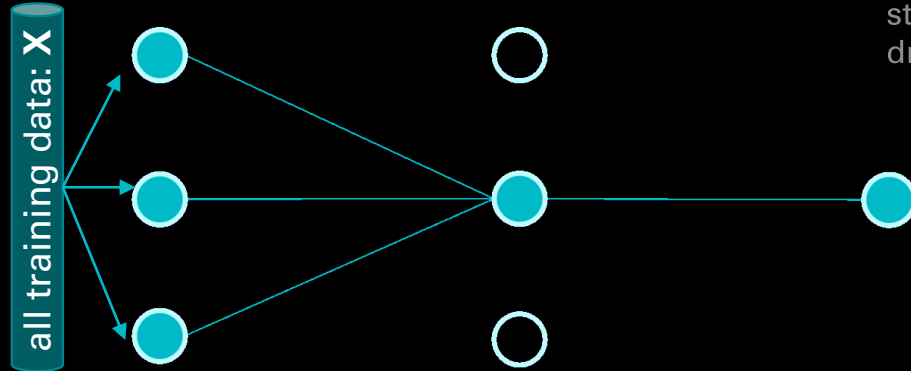
Sampling stochastic outputs => approximation to predictive posterior distribution



Methodology | MC Dropout

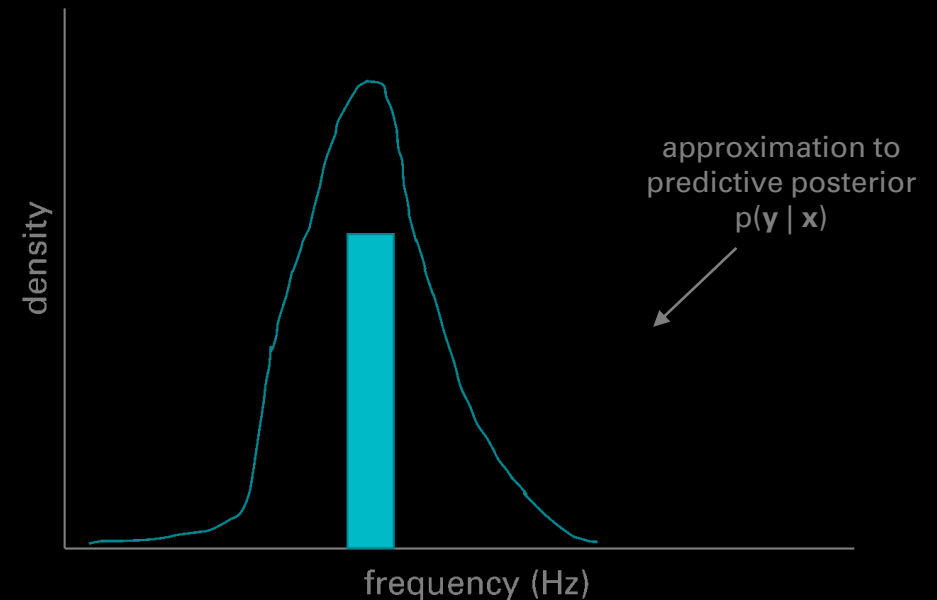
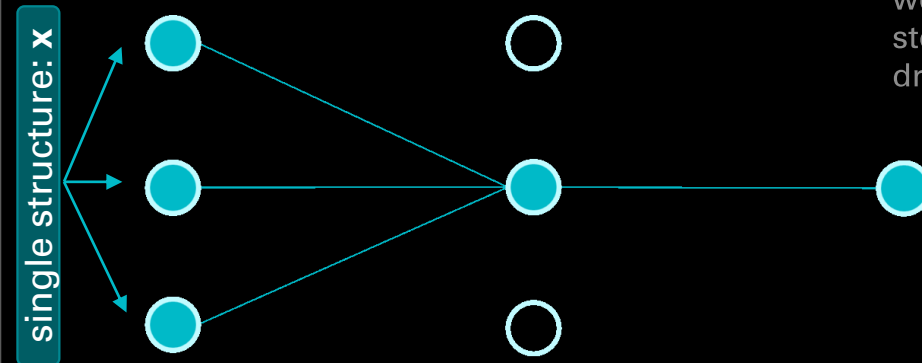
TRAINING

Learning weights + stochastic dropout



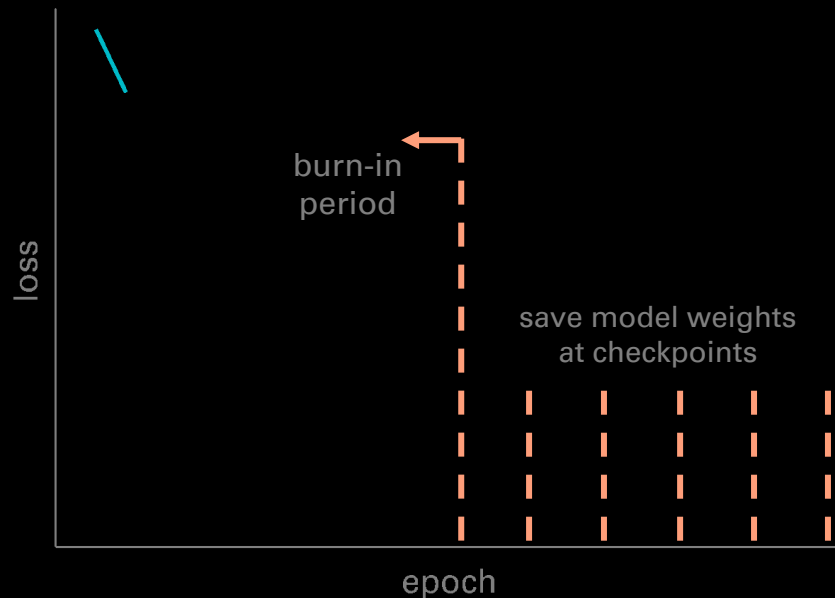
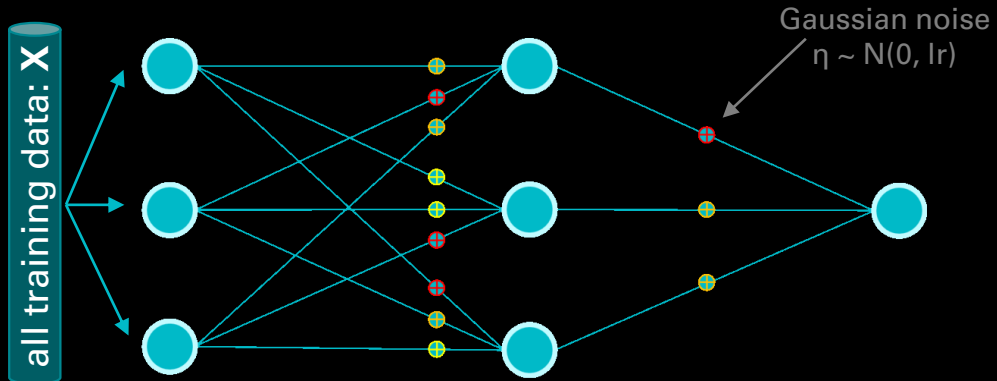
INFERENCE

Using learned weights + stochastic dropout

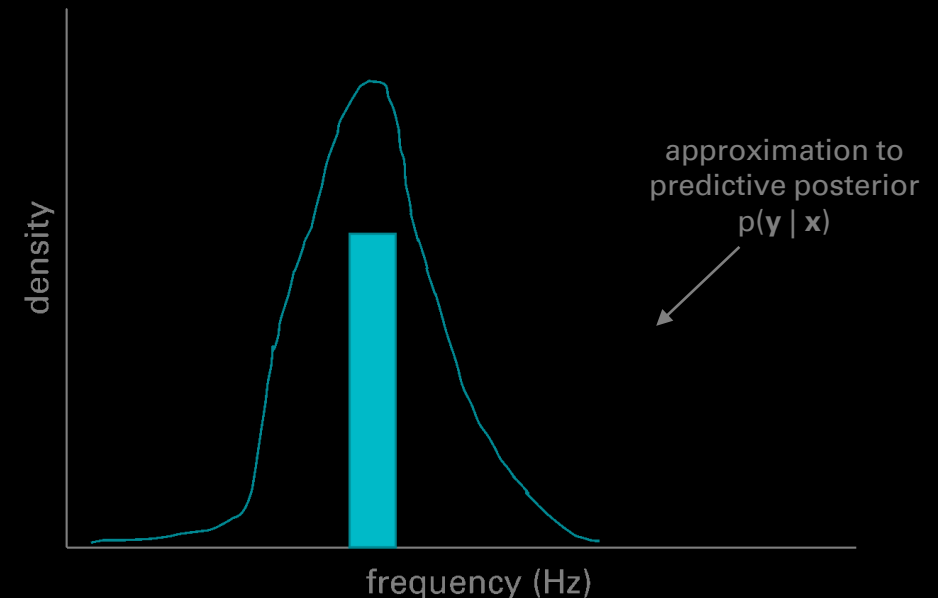
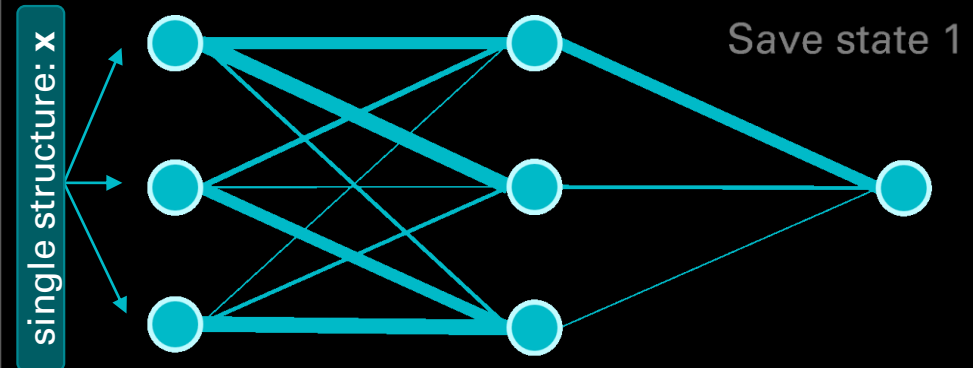


Methodology | Stochastic Gradient Langevin Dynamics (SGLD)

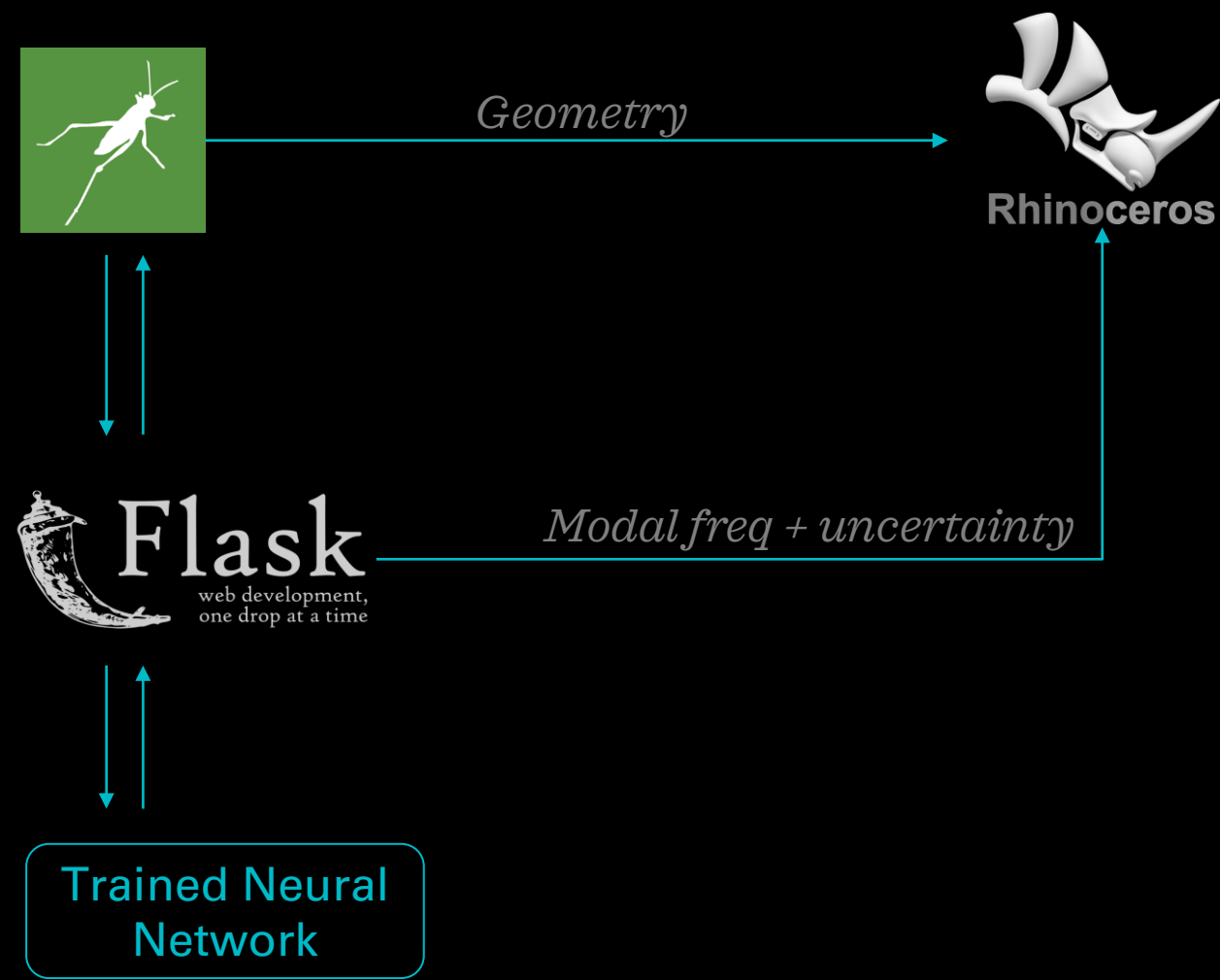
TRAINING



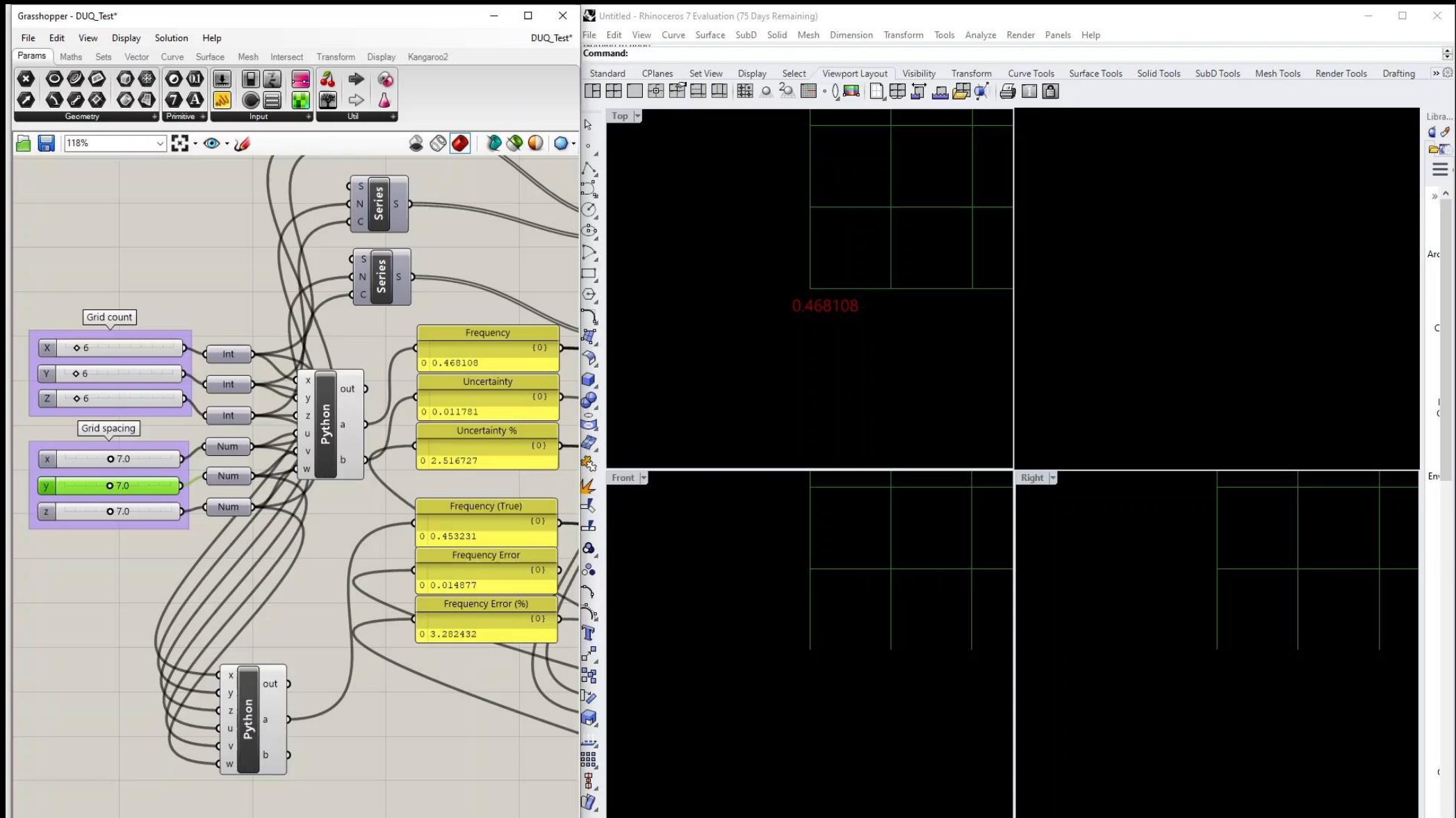
INFERENCE



Results | Visualising Uncertainty



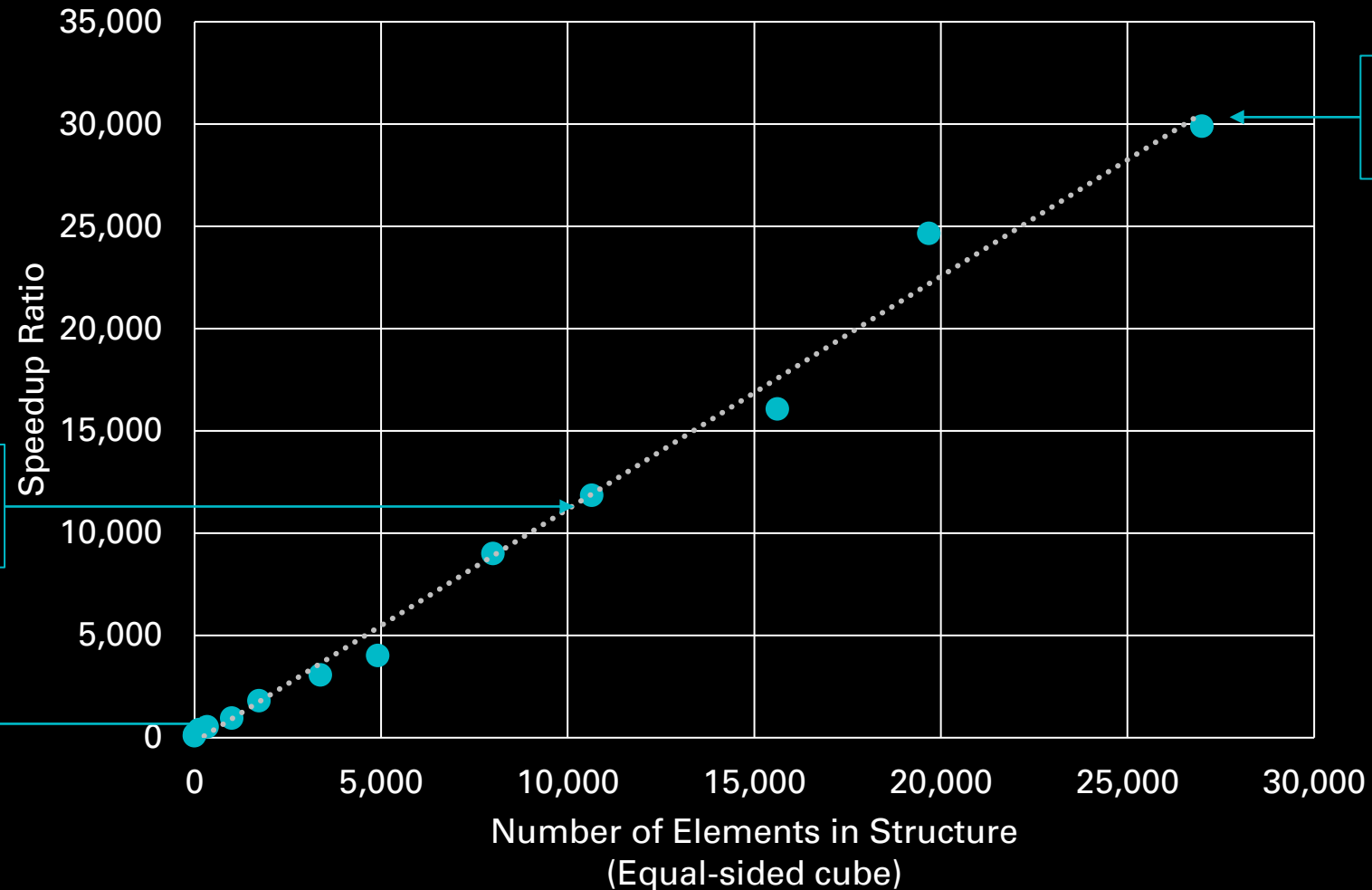
Results | Visualising Uncertainty – Grasshopper & Rhino



Results | Speed

Complexity Scaling:
GSA: $O(n)$
Surrogate: $O(1)$
 $n = \text{no. elements}$

Speedup Ratio:
Surrogate vs. GSA Analysis

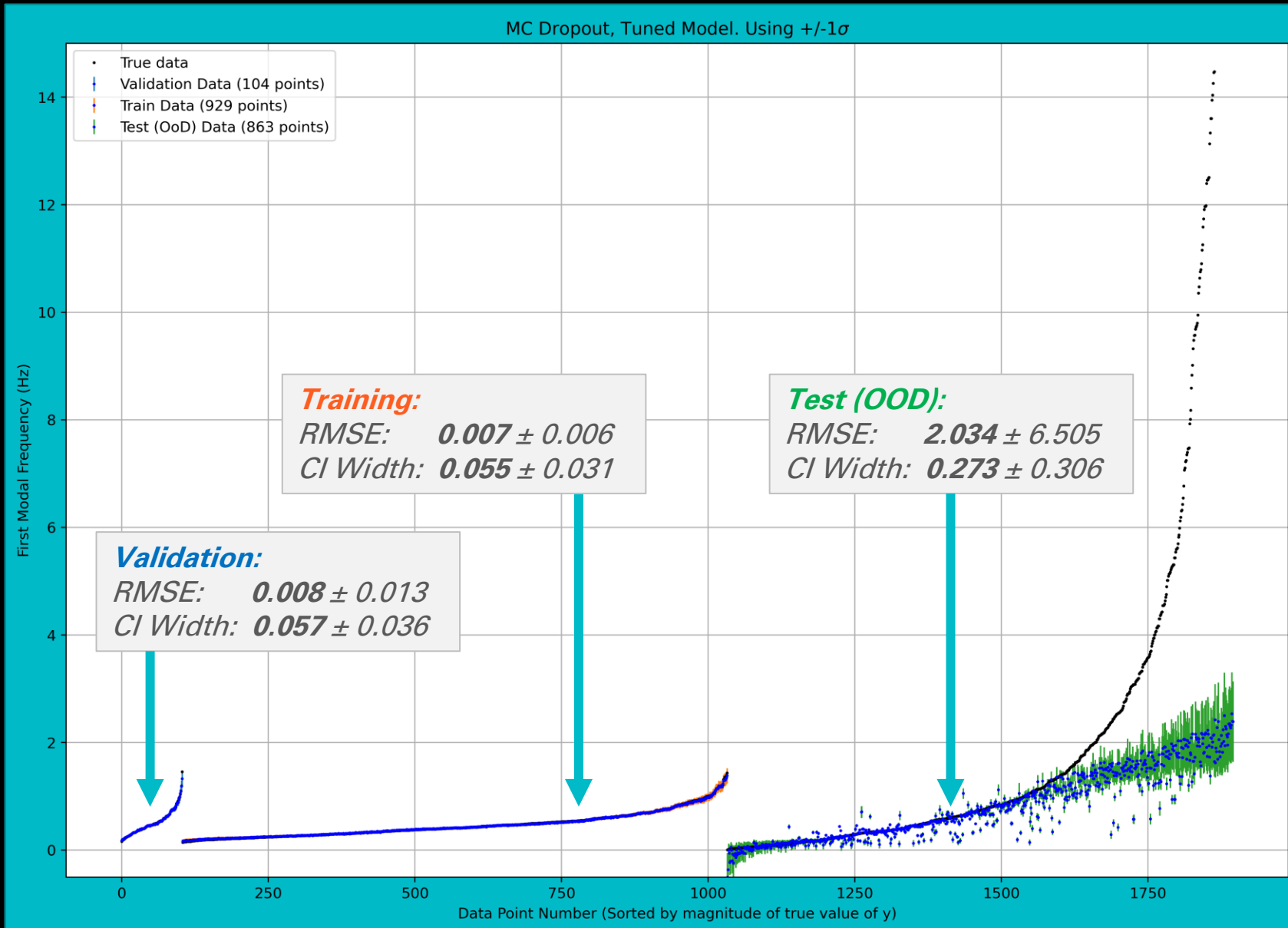


22x22x22:
11,000x speedup

5x5x5:
500x speedup

30x30x30:
28,000x speedup

Results | Accuracy and Uncertainty: Reference Datasets

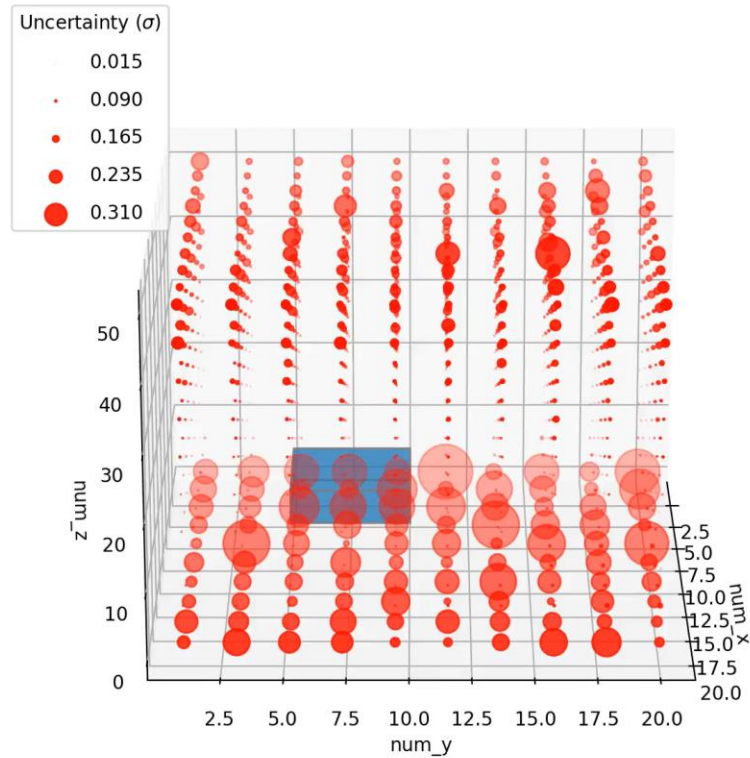


Results | Uncertainty - Unseen Geometries

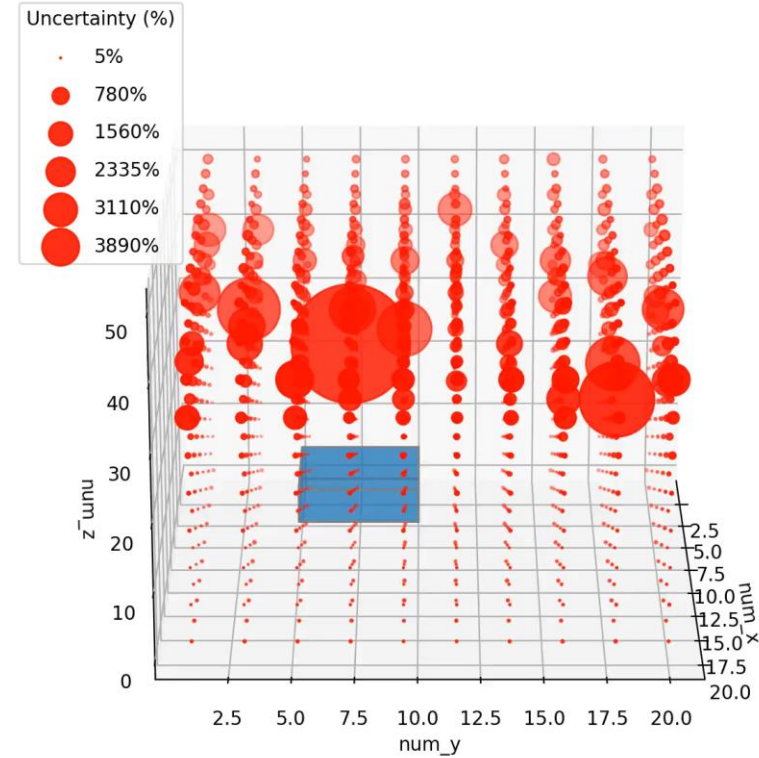
Fixed: length of elements in x , y , z

Varying: number of elements in x , y , z

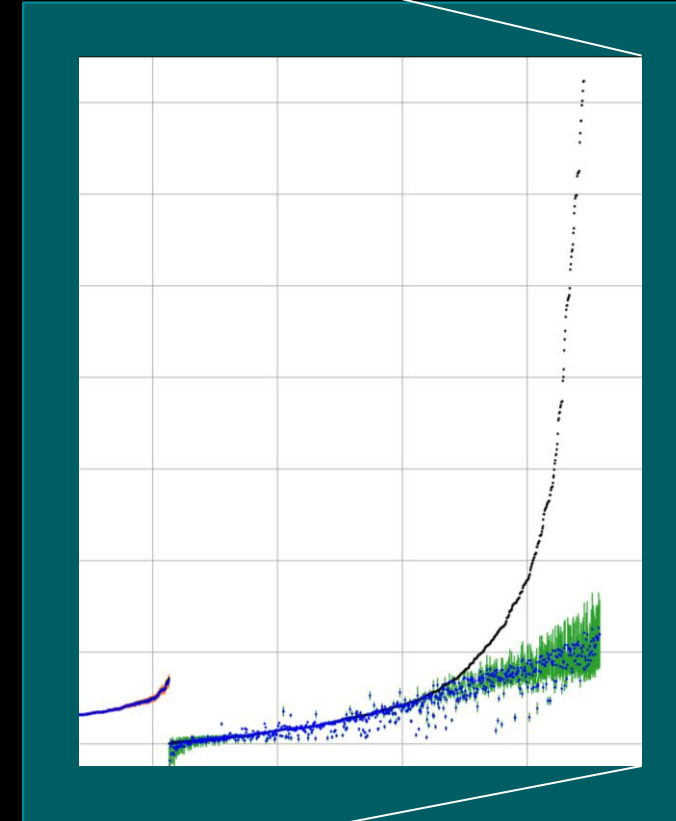
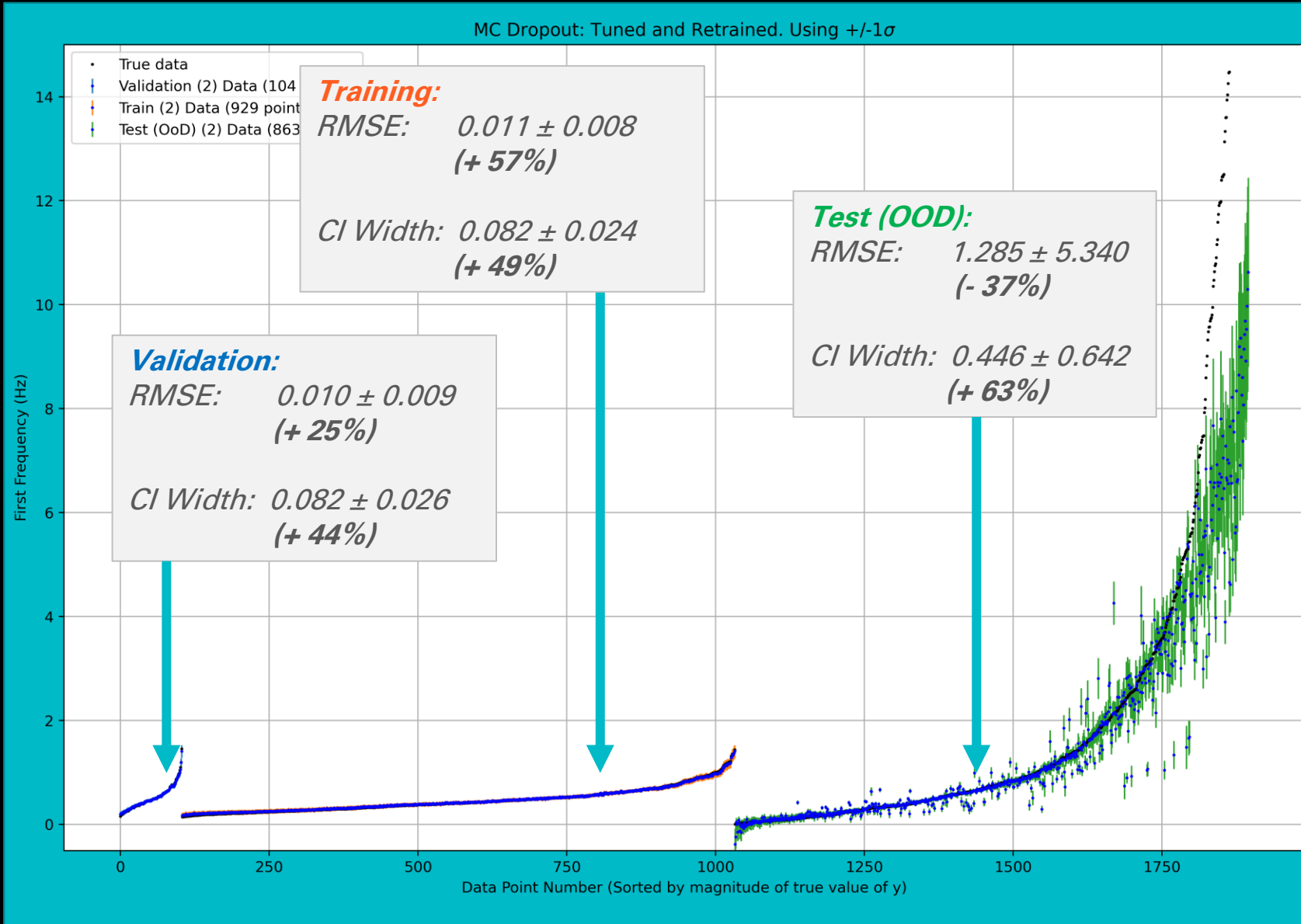
Absolute Uncertainty



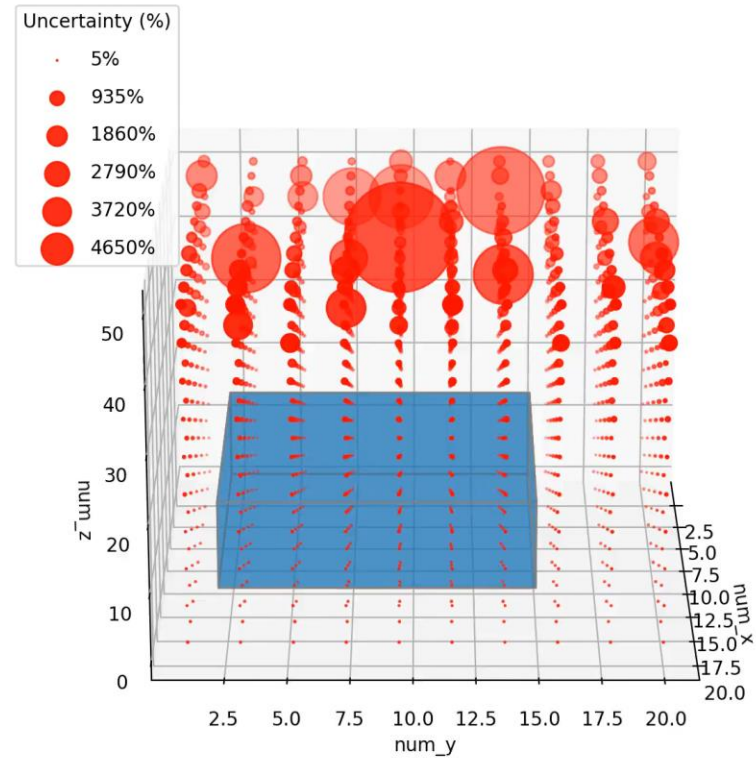
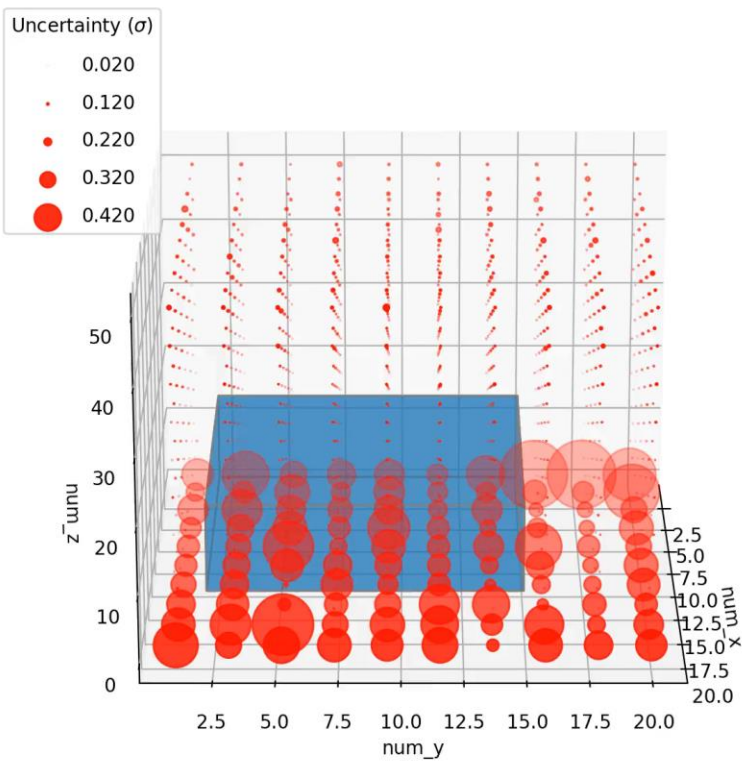
Relative (Percentage) Uncertainty



Results | Retraining With Additional Data



Results | Uncertainty - Unseen Geometries



Thank you for listening

Questions?