Parameter Space Exploration Using Simulations for Inspection Design and Qualification

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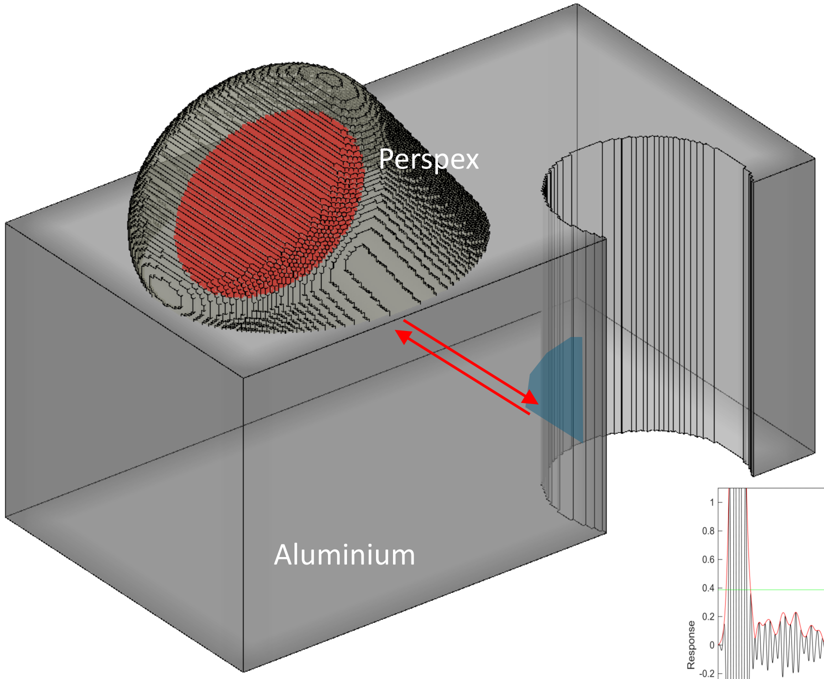
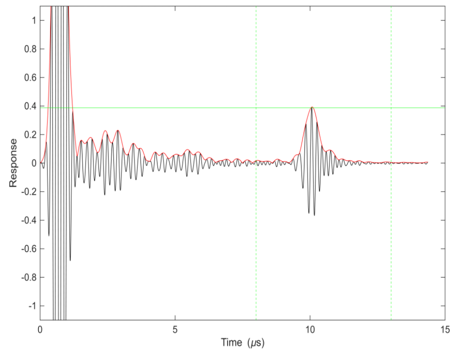
Context

- Full 3D FE simulations (e.g. Pogo) capturing all relevant physics are becoming viable



pogo.
www.pogo.software

~5mins on PC with standard GPU; main limitation on model size is GPU memory



- Assuming we have a validated, physics-based model (e.g. FE) that can accurately simulate any ultrasonic inspection, how do we use that model to design and qualify an inspection?
    - How do we know which cases to run?
    - How do we know when we have run enough?
    - How do we visualise and interpret the output?
    - How do we quantify uncertainty?

Context

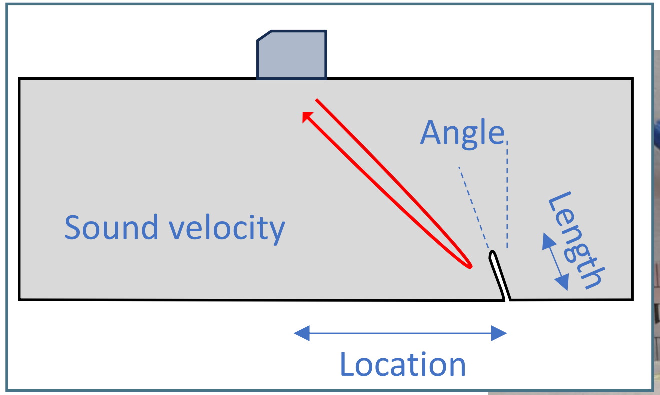
- ***Fast, efficient and reliable: digital qualification of ultrasonic inspection for safety-critical components*** – EPSRC/RCNDE-funded collaborative project between Imperial College and University of Bristol (Project Lead: Peter Huthwaite, Imperial)
  - WP1 – Bottom up – improving speed and accuracy of simulations (Imperial)
  - WP2 – Top down – making effective use of simulation results (Bristol)
  - WP3 – Integration and application (Imperial/Bristol)

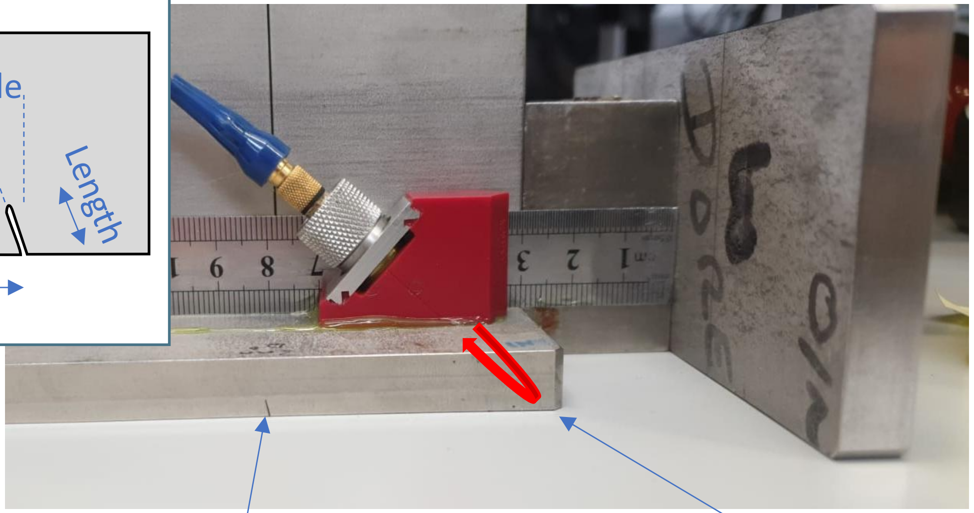
Outline

- Inspection example
  - FE model validation
- Generalised $\hat{a}$ vs. a approach – support for inspection qualification
  - Limitations of standard $\hat{a}$ vs. a approach
  - Methodology
  - Benefits of generalised approach
- Parameter space visualisation – support for inspection design
  - Parameter types
  - Methodology
  - Example
- DigiQual toolkit – software in progress

Inspection example

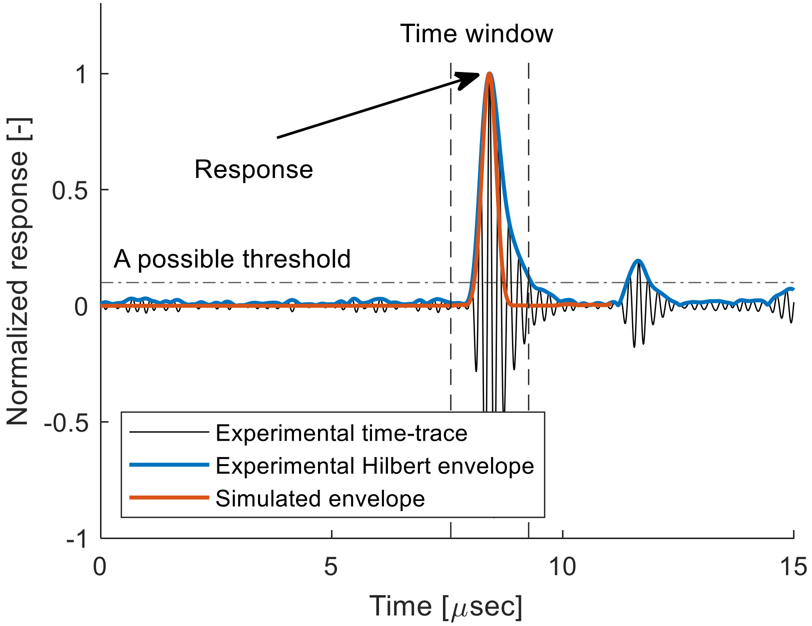
- Oblique incident shear wave inspection of surface-breaking cracks
  - 5MHz, 45° wedge, aluminium samples with s/breaking EDM notches





EDM crack (for experimental validation of model)

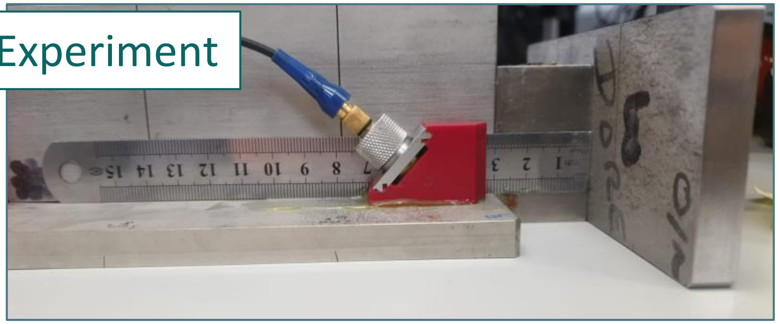
Corner (used to provide reference reflection in model and experiment)



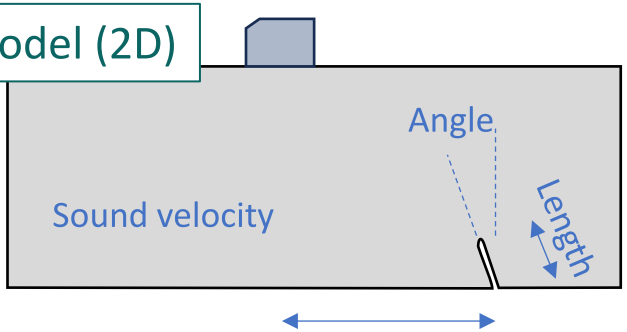
Inspection example – FE model validation

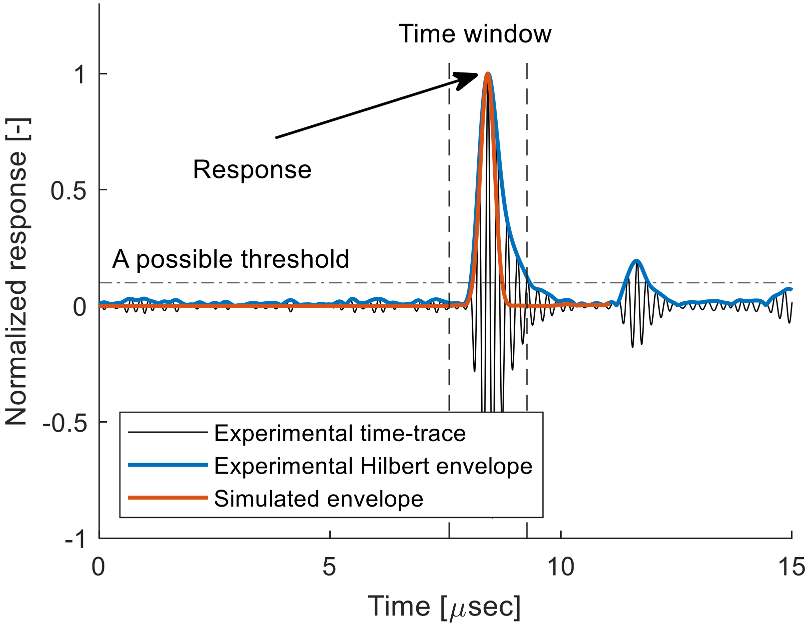
- Comparison of FE and experimental predictions of response from corner and two inclined cracks

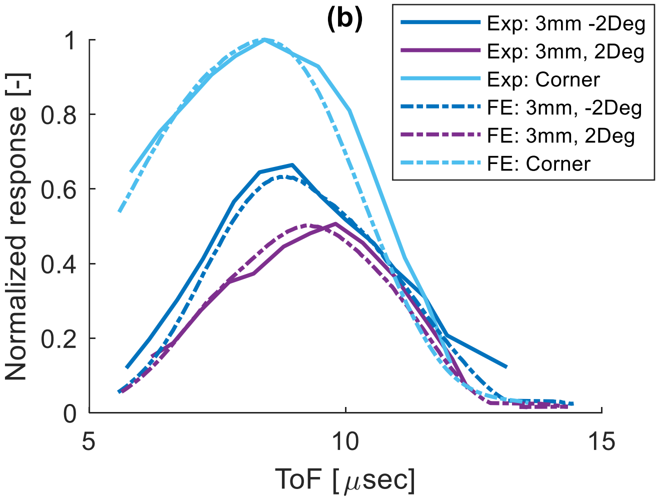
Experiment



FE model (2D)

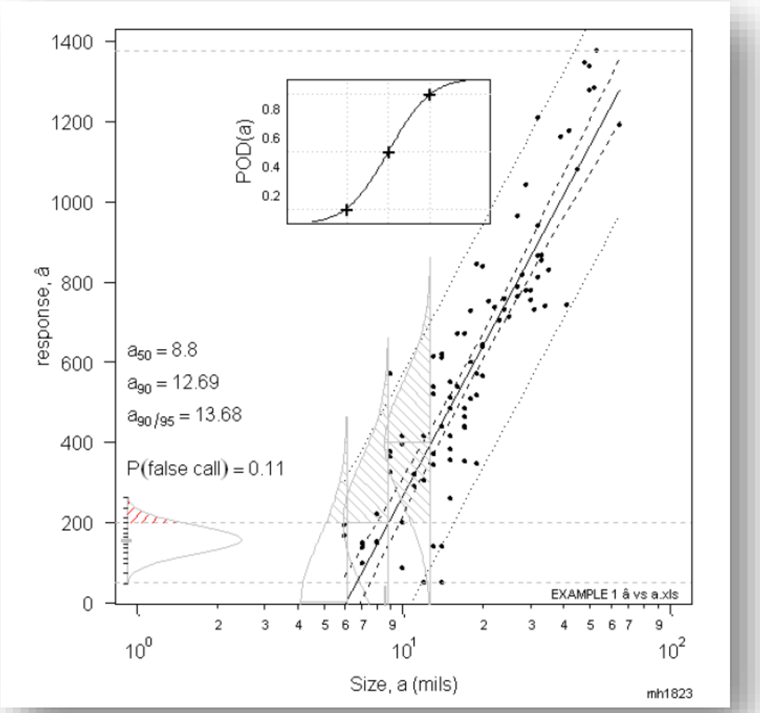






Generalised $\hat{a}$ vs. a approach

- Concept and limitations of <u>standard</u> $\hat{a}$ vs. a approach
  - Obtain responses ($\hat{a}$) for various defect sizes (a)
  - Transform one or both (e.g. $\hat{a} \rightarrow \log \hat{a}$) so relationship between $\hat{a}$ and a is as close to <u>linear</u> as possible
  - Assume points <u>normally distributed</u> about line of best fit with <u>constant variance</u> (due to other parameters)
  - Enables prediction of PoD vs. a with quantified uncertainty
  - Good for
    - Limited amount of data (typically ~100 experimental points)
    - Well-behaved inspection
    - Well-chosen representative data points
    - Data that satisfies <u>assumptions</u>!



Generalised $\hat{a}$ vs. a approach

- Physical models (e.g. FE) can efficiently provide many more data points than experiments
- Many examples of model-assisted PoD studies and surrogate modelling
- However, final PoD calculation and uncertainty quantification almost always based on standard $\hat{a}$ vs. a approach

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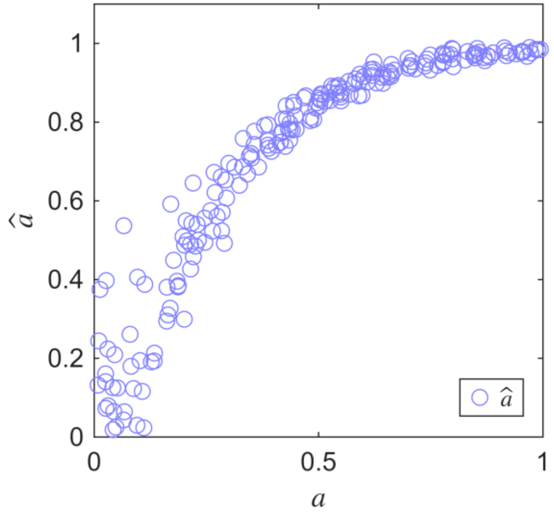
Generalised $\hat{a}$ vs. a approach

- Methodology – two-stage statistics
  - Fit first function (e.g. polynomial) to data points to describe mean, $\mu(a)$



Malkiel, Croxford, and Wilcox, “A generalized method for the reliability assessment of safety-critical inspection”, *Proc. Roy. Soc A*, 481, 2312, 2025

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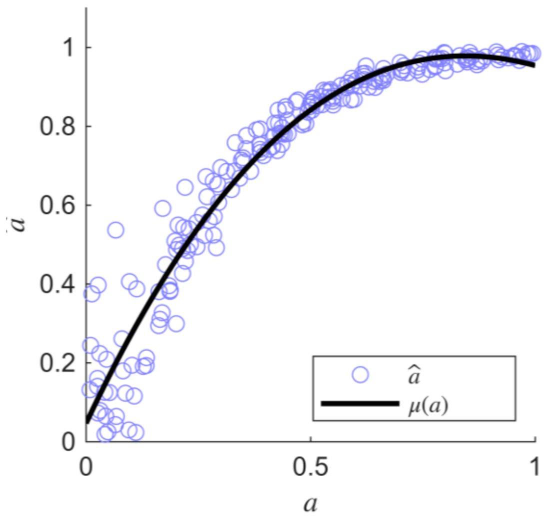

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Generalised $\hat{a}$ vs. a approach

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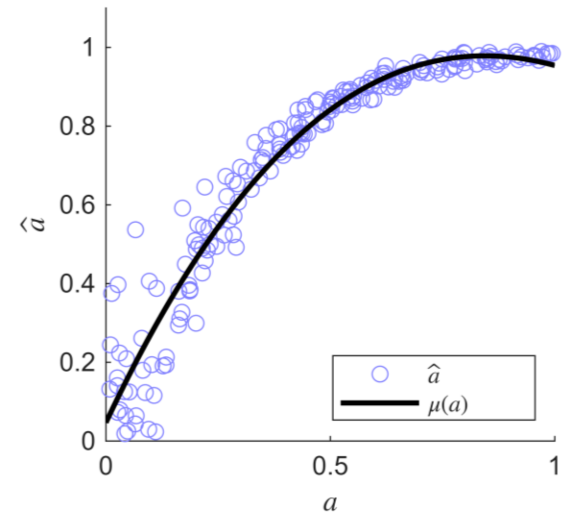
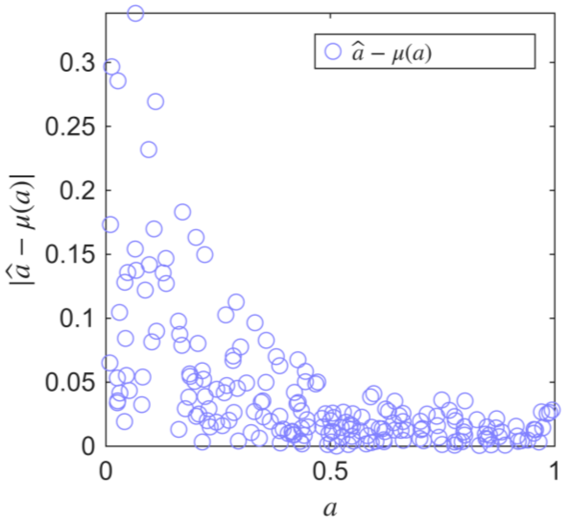
  - Fit first function (e.g. polynomial) to data points to describe mean, $\mu(a)$
  - Compute error $|\hat{a} - \mu(a)|$ between each data point and mean





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Generalised $\hat{a}$ vs. a approach

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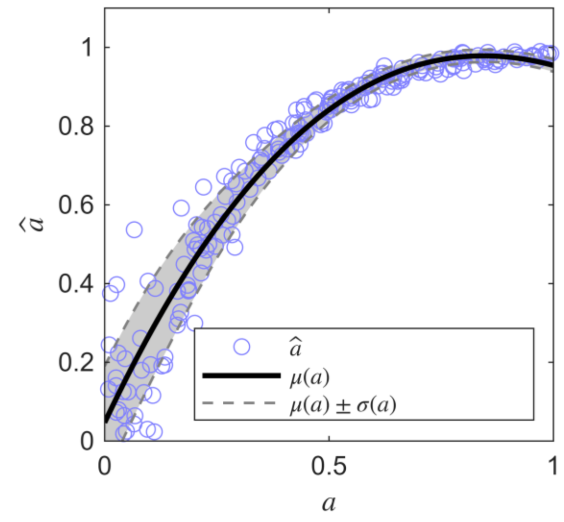
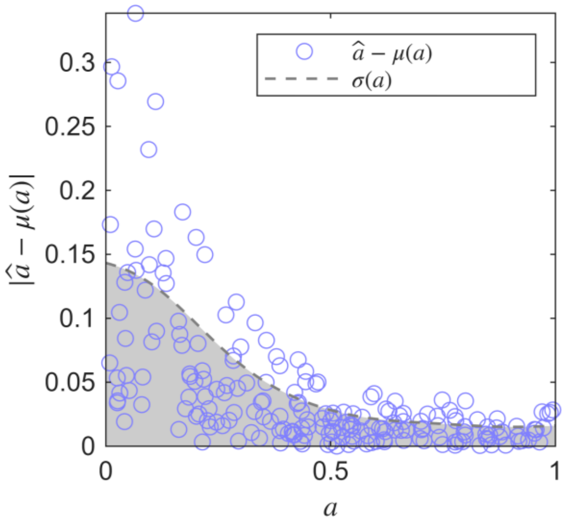
  - Fit first function (e.g. polynomial) to data points to describe mean, $\mu(a)$
  - Compute error $|\hat{a} - \mu(a)|$ between each data point and mean
  - Fit second function to $|\hat{a} - \mu(a)|$ to get standard deviation, $\sigma(a)$





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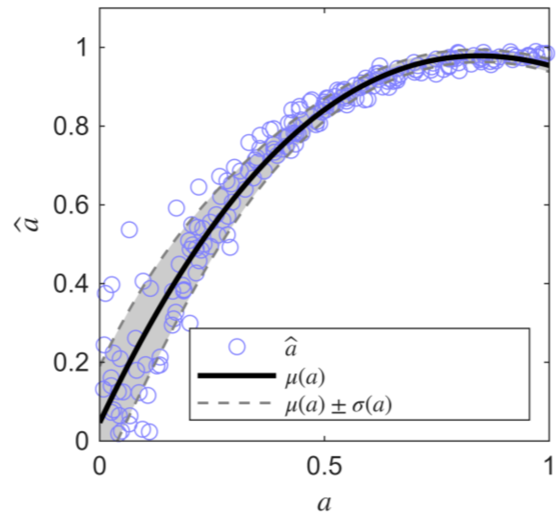
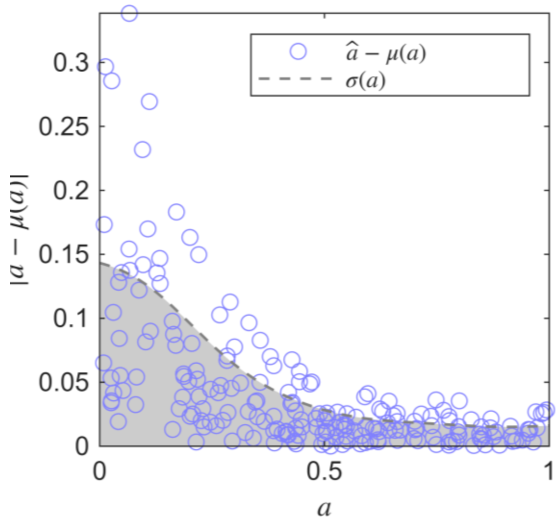
Generalised $\hat{a}$ vs. a approach

- Methodology – two-stage statistics
  - Fit first function (e.g. polynomial) to data points to describe mean, $\mu(a)$
  - Compute error $|\hat{a} - \mu(a)|$ between each data point and mean
  - Fit second function to $|\hat{a} - \mu(a)|$ to get standard deviation, $\sigma(a)$
  - Test candidate statistical distributions (e.g. Gaussian, Gumbel-min) and select most-likely, $f(a; \mu(a), \sigma(a))$
    - PoD(a) curve for given threshold computed analytically from $f(a; \mu(a), \sigma(a))$
    - PoD(a) confidence interval computed by bootstrapping





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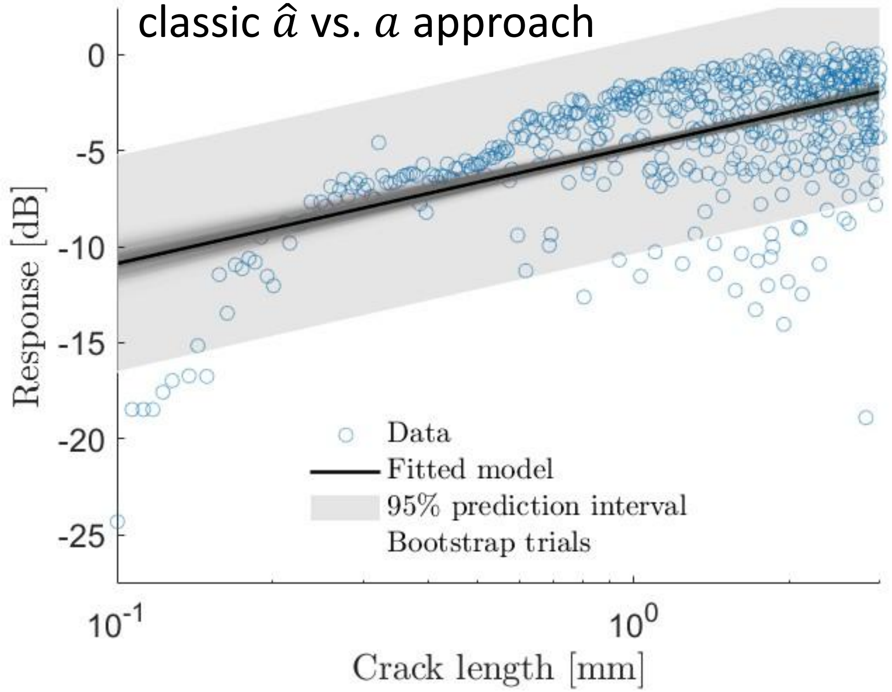
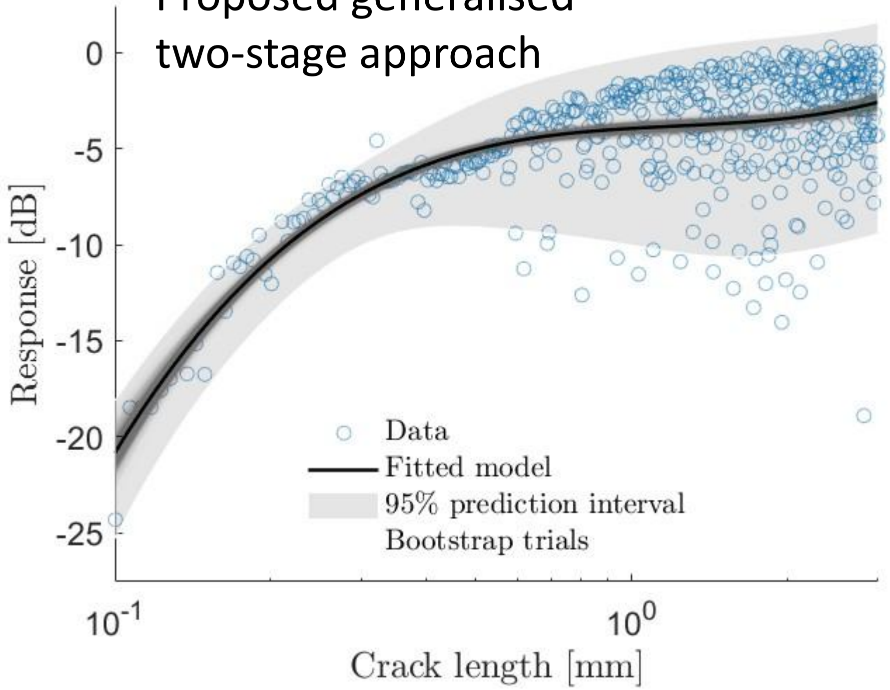
Generalised $\hat{a}$ vs. a approach

- Avoids limiting assumptions of standard $\hat{a}$ vs. a approach
  - Handles non-linear response with non-uniform variance
  - Two-stage statistics enabled by increased number of data points (500 here)

Best you can get from classic $\hat{a}$ vs. a approach



Proposed generalised two-stage approach



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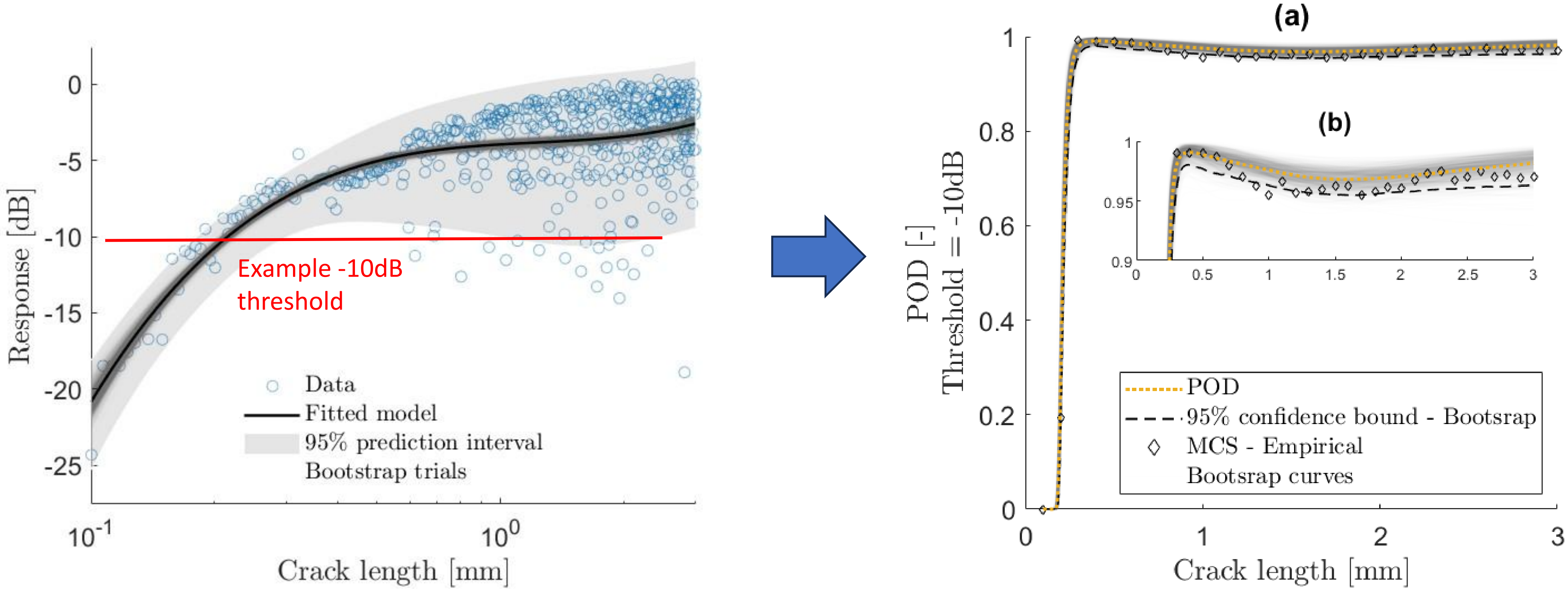
Generalised $\hat{a}$ vs. a approach

- Example output: response curve and PoD curve with uncertainty



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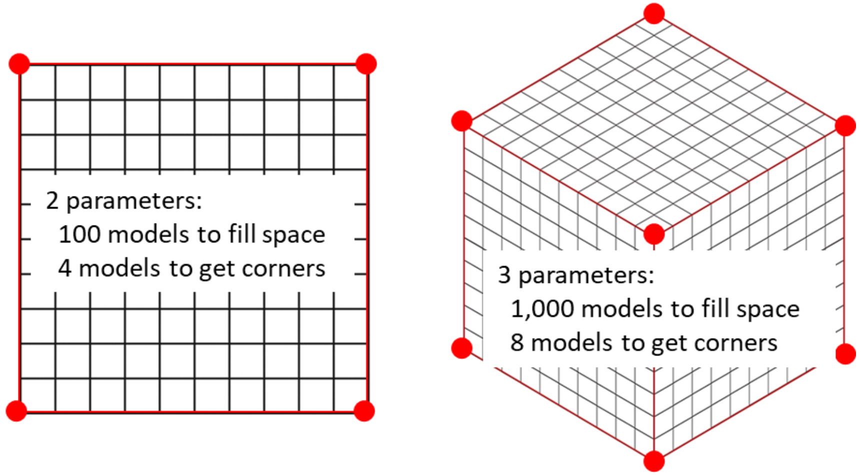
Parameter space visualisation

- Generalised $\hat{a}$ vs. a approach can deal with many parameters, but response is presented as stochastic function of one parameter
- Why visualise effect of multiple parameters?
  - Better understanding of inspection / improved design
  - Identification of worst-case scenarios (e.g. for experimental trials)
- Challenges
  - Efficiently obtaining response functions of multiple parameters from limited simulations



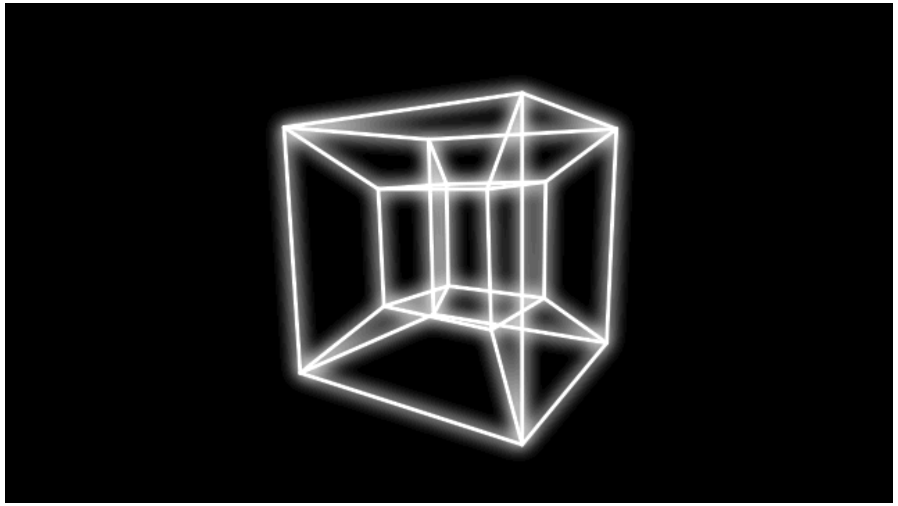
10 parameters:

10^{10} = 10,000,000,000 models to fill space!

2^{10} = 1,024 models needed just to get corners of parameter space

Parameter space visualisation

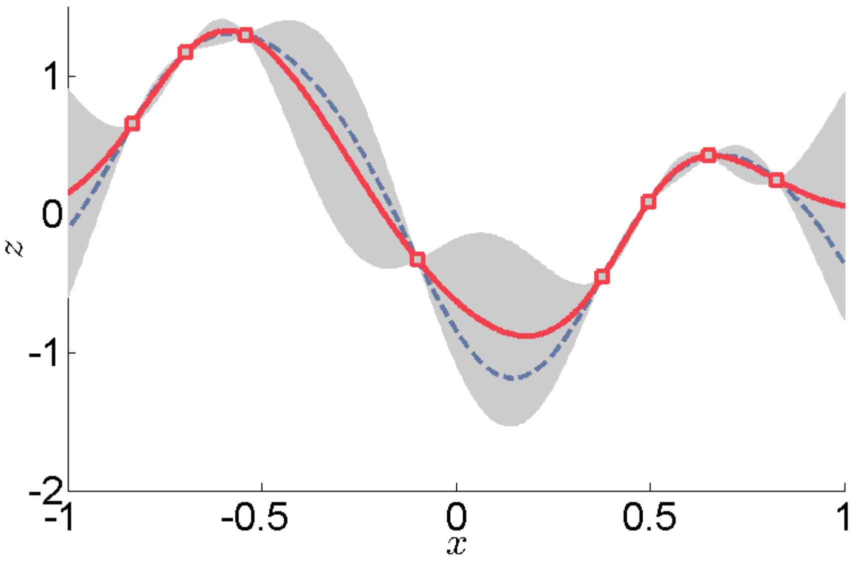
- Generalised $\hat{a}$ vs. a approach can deal with many parameters, but response is presented as stochastic function of one parameter
- Why visualise effect of multiple parameters?
  - Better understanding of inspection / improved design
  - Identification of worst-case scenarios (e.g. for experimental trials)
- Challenges
  - Visualisation of response functions of $n > 2$ parameters



Parameter space visualisation

- Methodology – Kriging surrogate model
  - Interpolates (multi-dimensional) response function between FE data points
  - Provides mean and variance of interpolation at all points
  - Space-filling algorithm to decide parameters for FE model executions
  - Iterative scheme to do FE simulations until surrogate model achieves desired interpolation accuracy

1D visualisation of Kriging



Data point (FE model result)
Most-likely interpolation
Interpolation confidence interval
Example of another possible (less likely) interpolation

[Wikipedia graphic]

Malkiel, Croxford, and Wilcox, "A comprehensive investigation of flexible and multi-dimensional simulation-based PoD analysis", *NDT&E Int.*, 2026

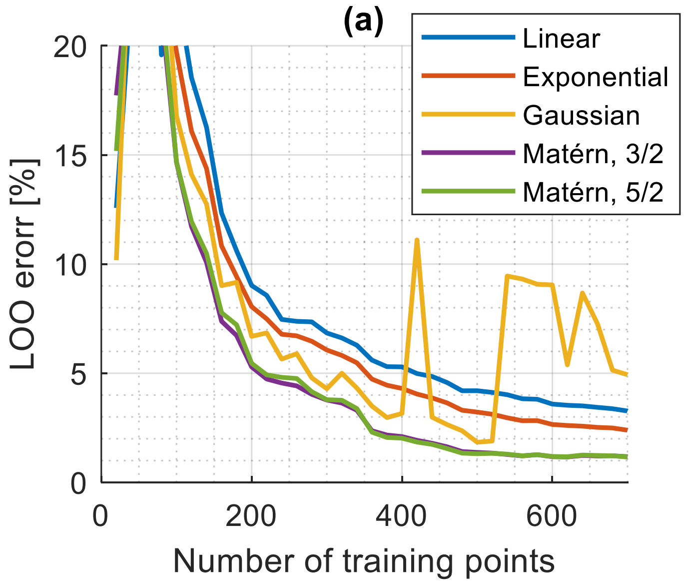
Parameter space visualisation

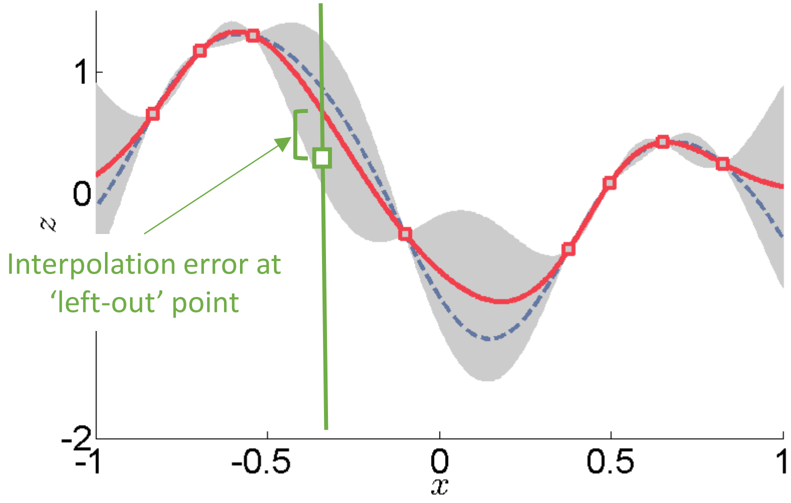
- Methodology – Fast Kriging surrogate model enables:
  - Quick ‘slicing’ of high-dimensional response function for visualisation and inspection design
  - Quick numerical integration of response function over nuisance dimensions to obtain PoD curves as functions of parameter(s) of interest
  - Uncertainty quantification of response function and PoD curves

Malkiel, Croxford, and Wilcox, “A comprehensive investigation of flexible and multi-dimensional simulation-based PoD analysis”, *NDT&E Int.*, 2026

Parameter space visualisation

- Methodology – tracking convergence
  - Leave-one-out (LOO) – perform fitting missing out one data point (□) and compare fitted value to actual value at missing point; repeat with every point missed out in turn





□ Data points used for interpolation

— Most-likely interpolation through □

□ ‘Left-out’ data point

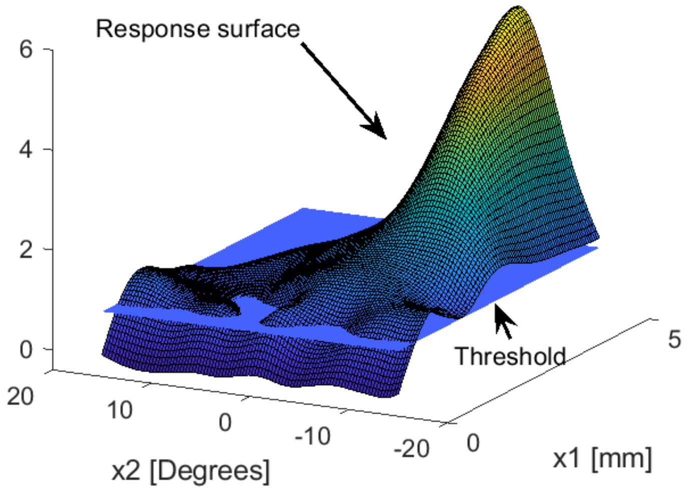
[Wikipedia graphic]

Malkiel, Croxford, and Wilcox, “A comprehensive investigation of flexible and multi-dimensional simulation-based PoD analysis”, *NDT&E Int.*, 2026

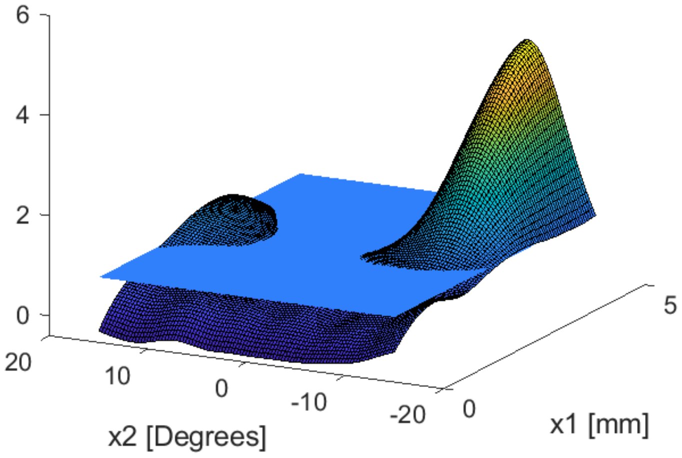
Parameter space visualisation – Slicing example

- 2D depth-angle slices through 4D response function for various arbitrary fixed values of crack position and shear velocity

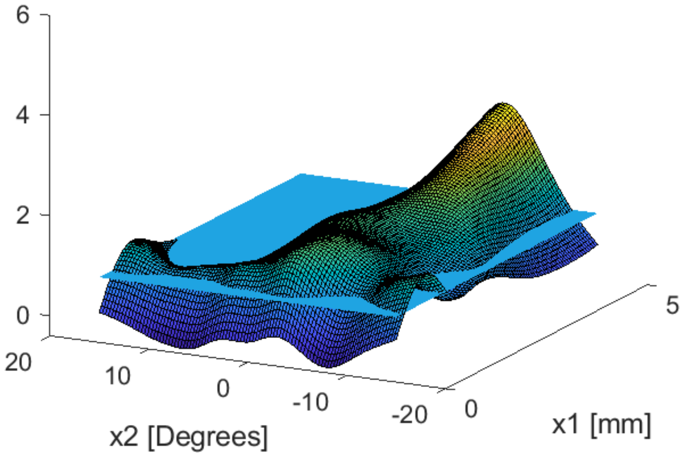
Position = 15.5 mm
Shear velocity = 3.250 mmμs^{-1}



Position = 13.5 mm
Shear velocity = 3.315 mmμs^{-1}



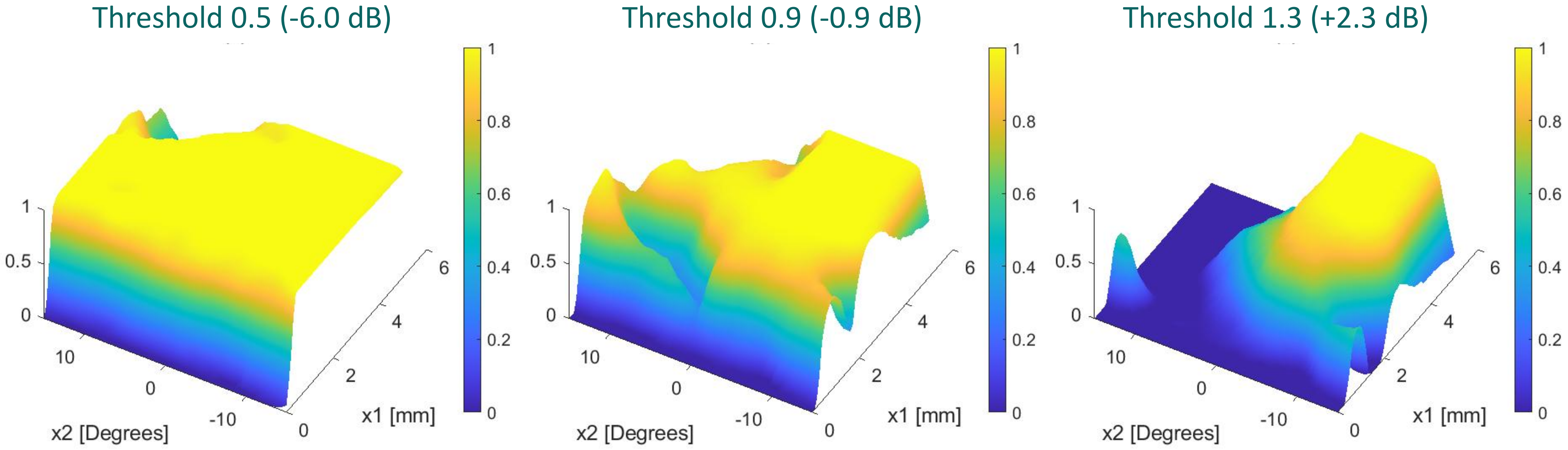
Position = 17.5 mm
Shear velocity = 3.185 mmμs^{-1}



Malkiel, Croxford, and Wilcox, “A comprehensive investigation of flexible and multi-dimensional simulation-based PoD analysis”, *NDT&E Int.*, 2026

Parameter space visualisation – Integration example

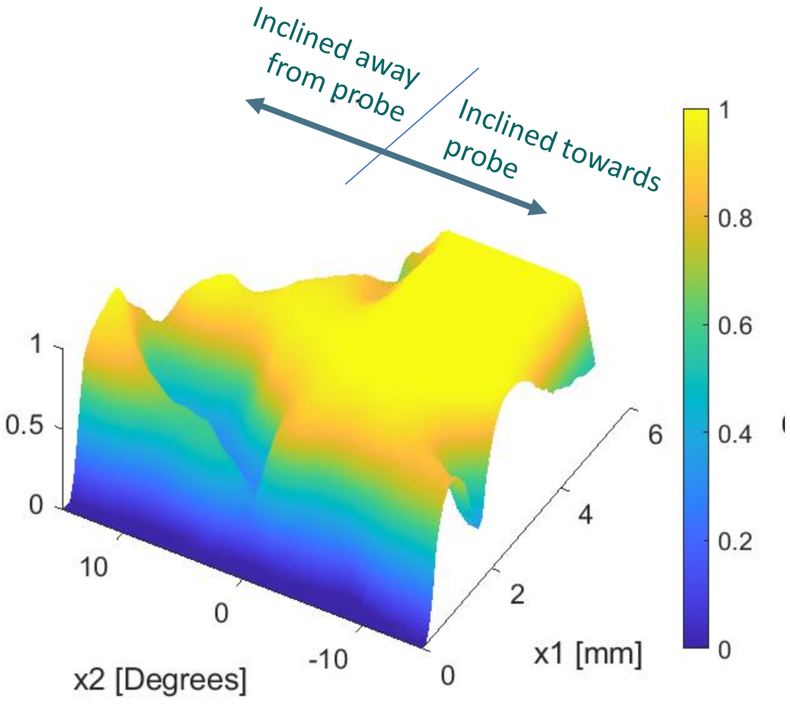
- Integration over other dimensions (crack position and shear velocity) of fraction of response > threshold gives PoD curve (2D surface)



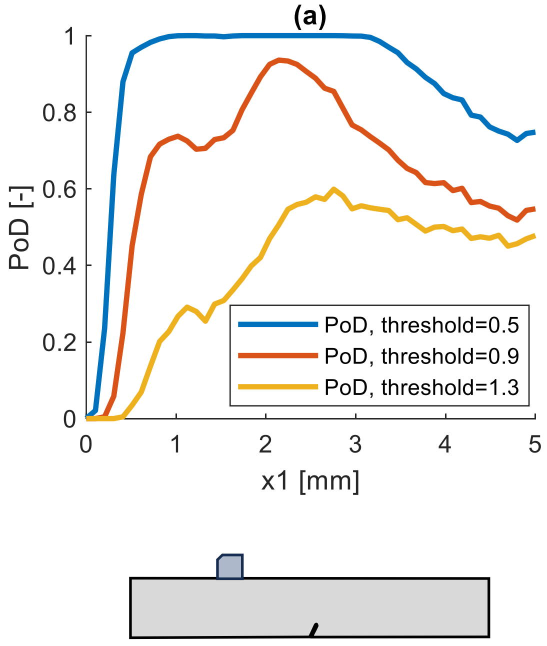
Malkiel, Croxford, and Wilcox, "A comprehensive investigation of flexible and multi-dimensional simulation-based PoD analysis", *NDT&E Int.*, 2026

Parameter space visualisation – Integration example

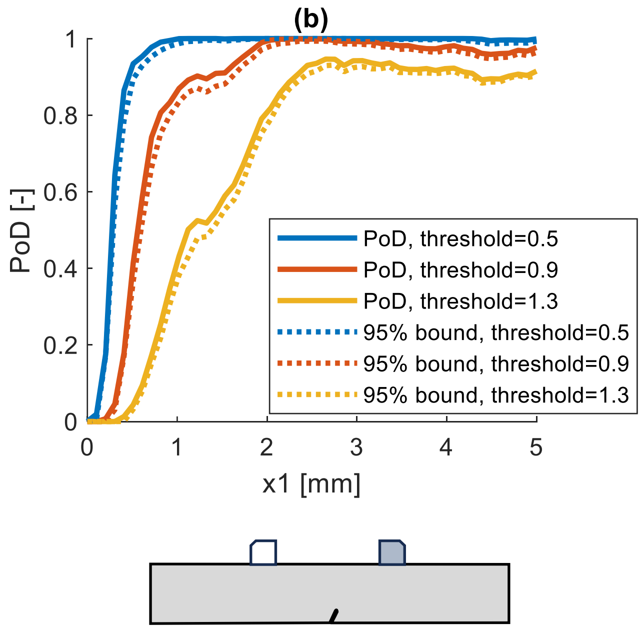
- Further integration to 1D PoD function of crack length
  - Shows effect of single- vs. double-sided access



Angle range [-15°, 15°] (single-sided access)



Angle range [-15°, 0°] (double-sided access)



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DigiQual toolkit – work in progress

- Concept
  - Python library for expert users to fully automate simulation workflow
    - Automatically select parameters for simulations
    - Automatically execute simulation using user's simulation tool*
    - Extract response of interest from simulation output*
    - Iteratively execute simulations and to achieved desired level of accuracy
    - Analyse responses and produce results with quantified uncertainty

  - GUI wrapper to inform simulations and analyse results
    - Produce table of parameters for simulation executions
    - *[User executes simulations and extracts responses of interest]*
    - Analyse responses and produce results with quantified uncertainty

*requires user to write script that runs simulation tool with given parameters and processes output

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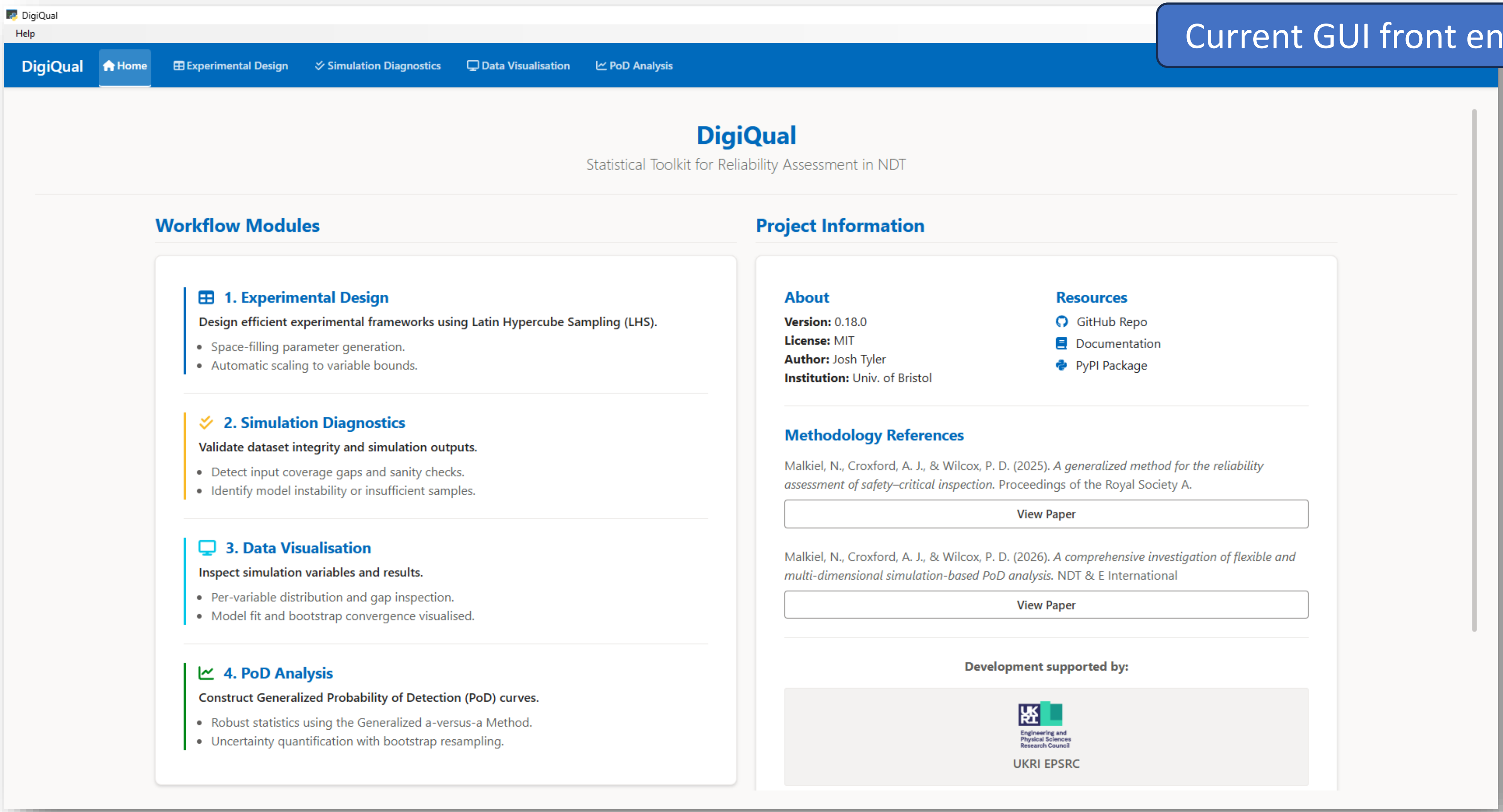
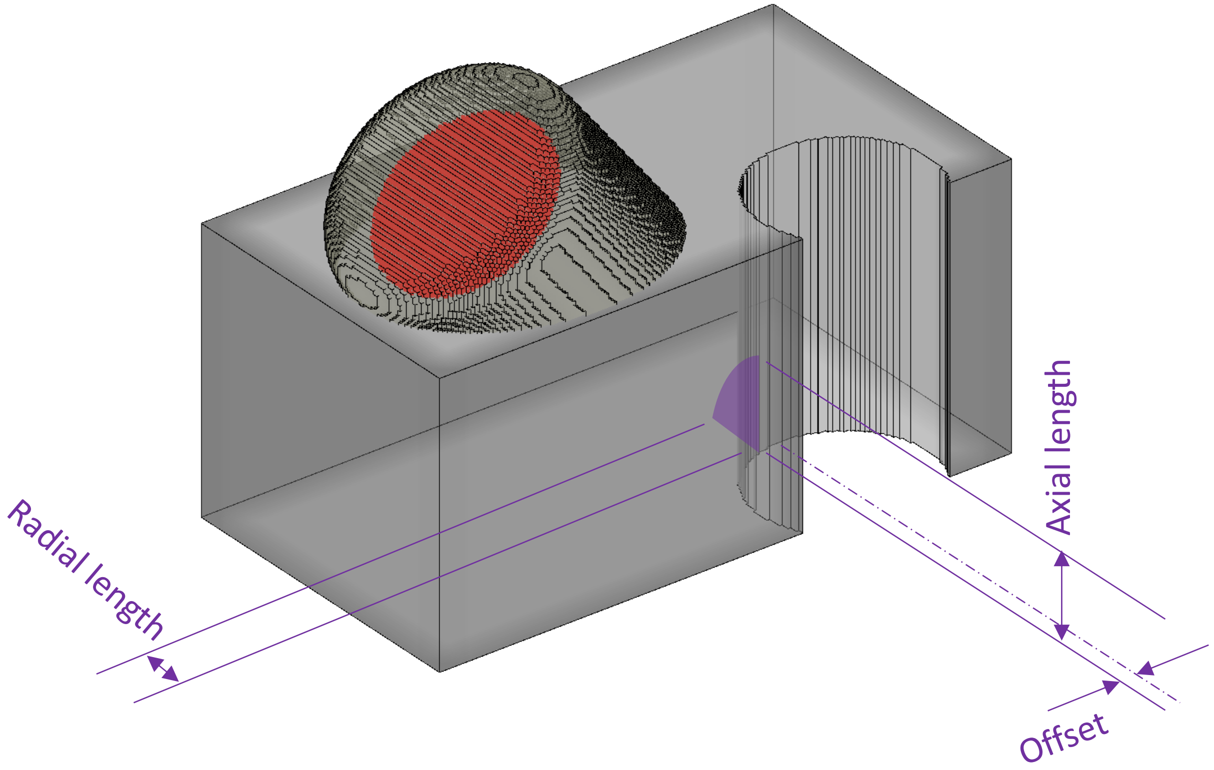
DigiQual toolkit – work in progress

Current GUI front end



DigiQual toolkit – work in progress

- Example – radial crack at fastener hole



DigiQual toolkit – work in progress

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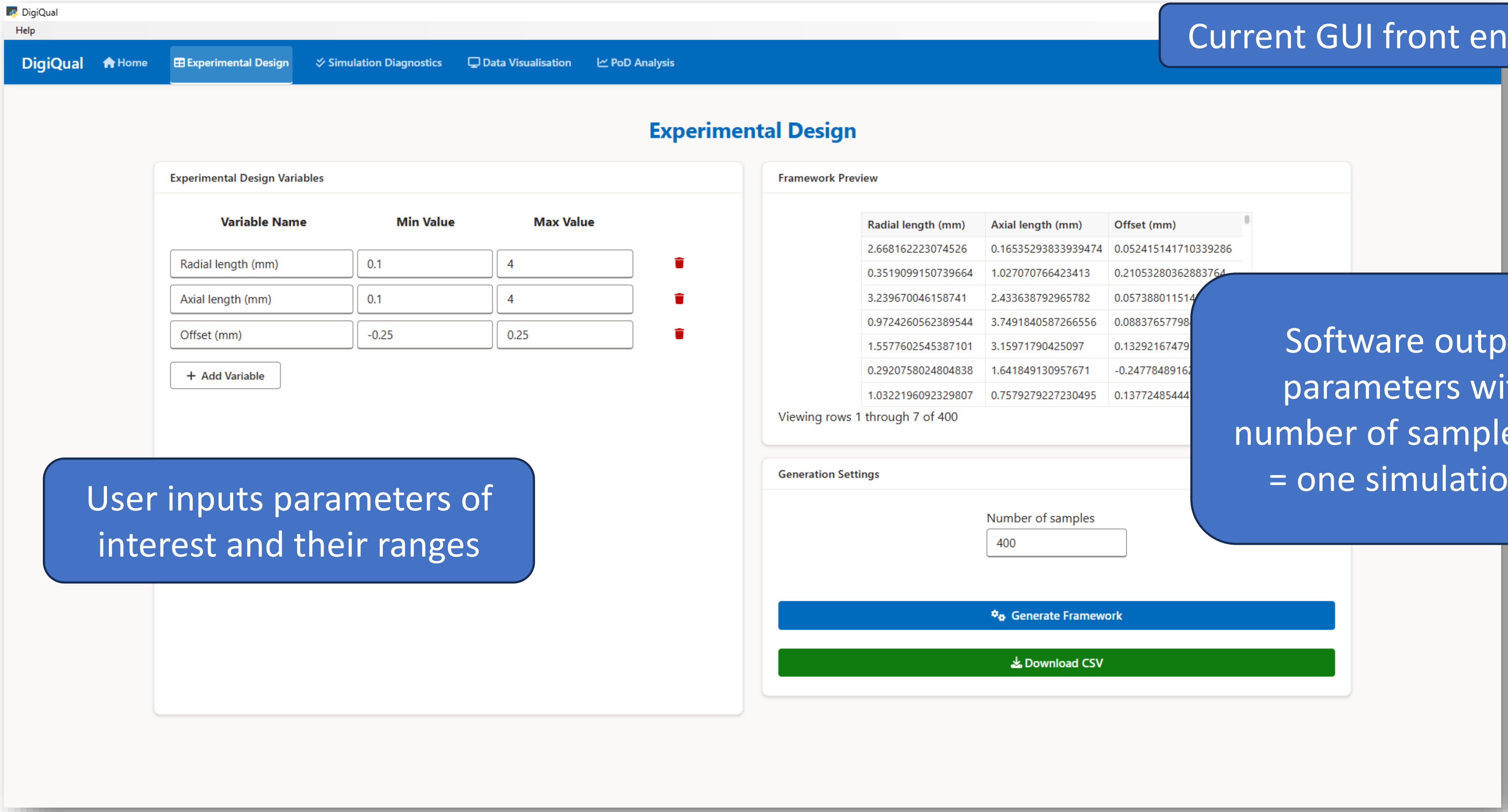
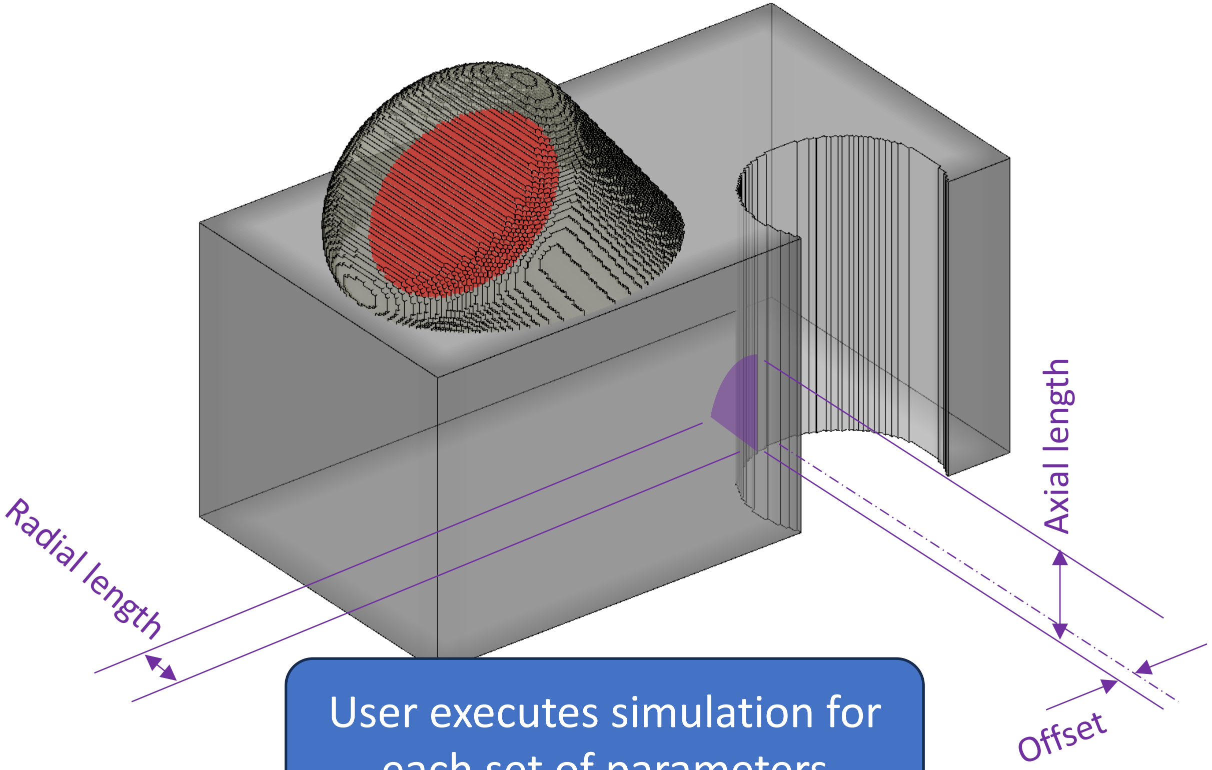


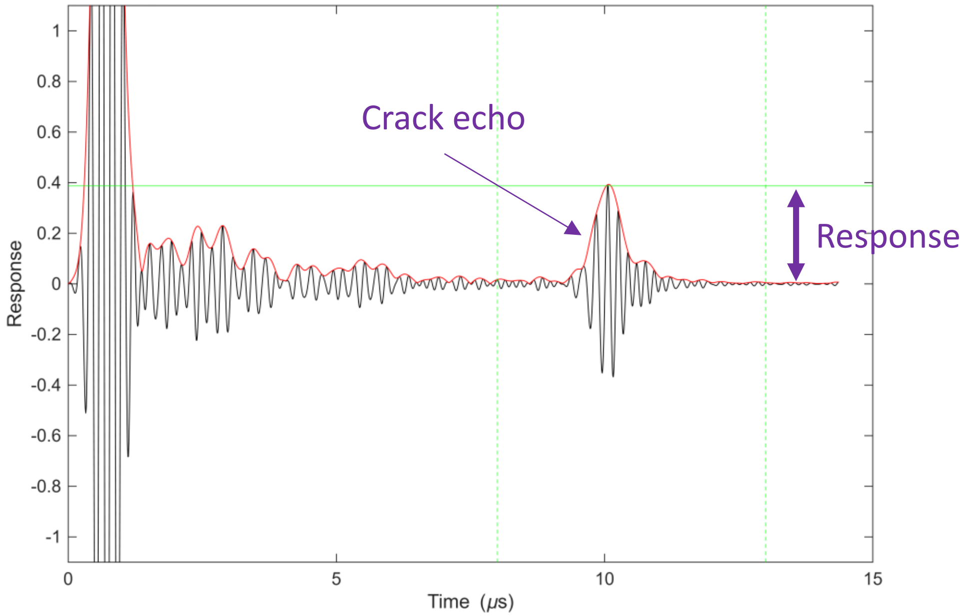
User inputs parameters of interest and their ranges

Software outputs table of parameters with specified number of samples (one sample = one simulation execution)

DigiQual toolkit – work in progress



User executes simulation for each set of parameters

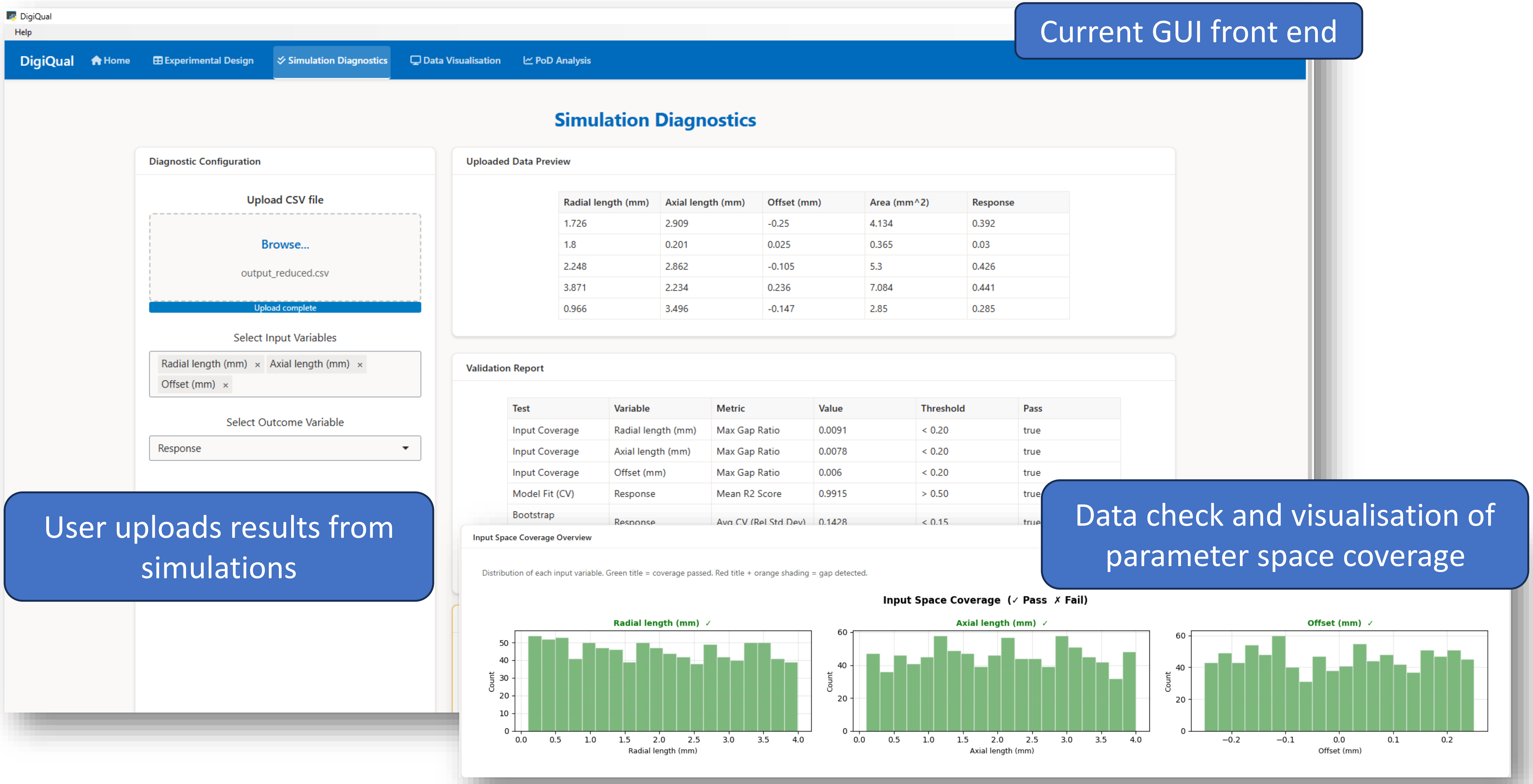


User extracts defect response from each simulation

pogo.
www.pogo.software

DigiQual toolkit – work in progress

Current GUI front end

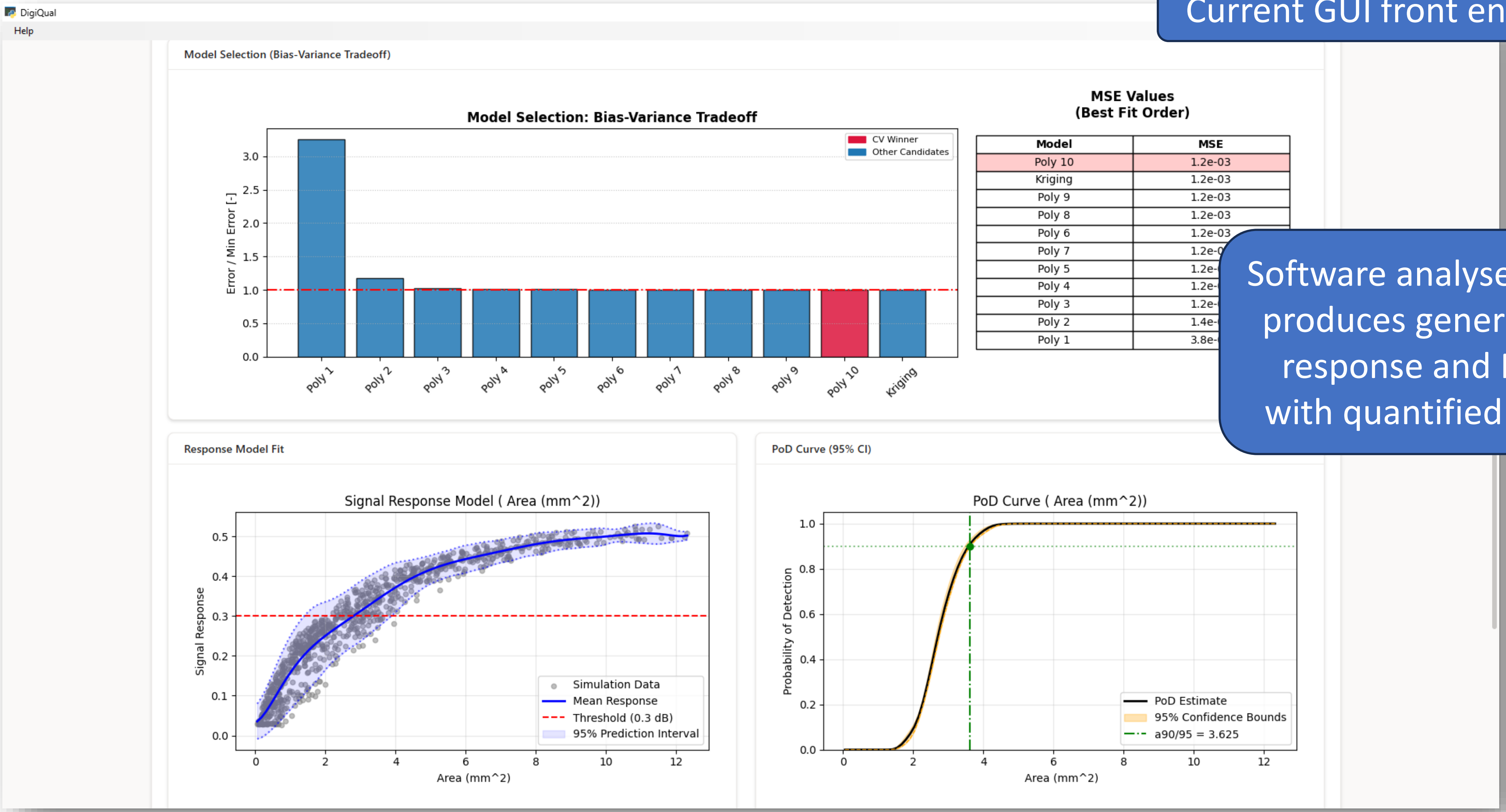


User uploads results from simulations

Data check and visualisation of parameter space coverage

DigiQual toolkit – work in progress

Current GUI front end



Software analyses results and produces generalised signal response and PoD curves with quantified uncertainty

Response model and PoD as function of 1 parameter

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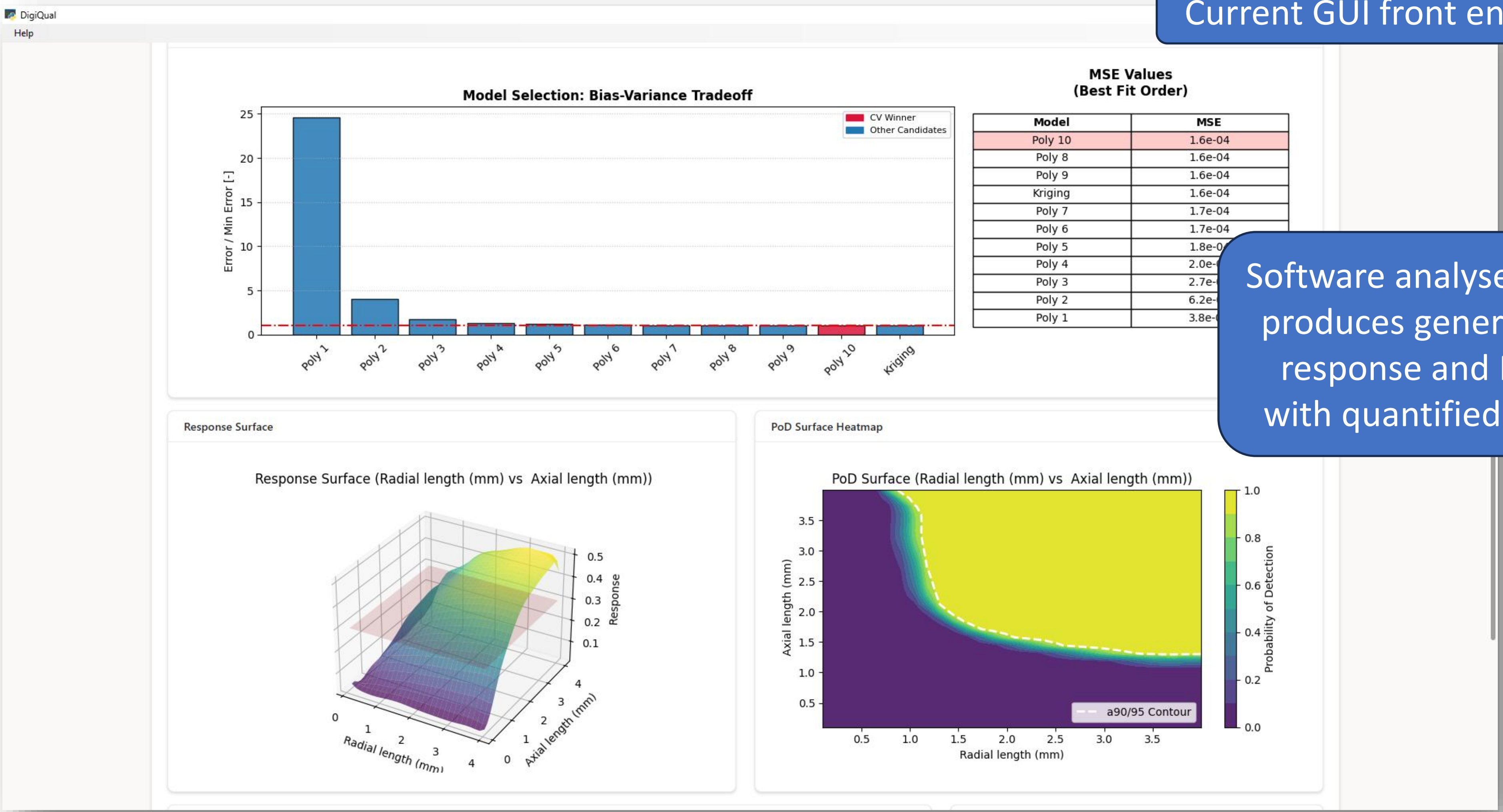
DigiQual toolkit – work in progress

Current GUI front end



Software analyses results and produces generalised signal response and PoD curves with quantified uncertainty

Response model and PoD as function of 2 parameters

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https://forms.office.com/e/pFDGgqpuJ8

DigiQual software survey

Background
The project *Fast, efficient and reliable: digital qualification of ultrasonic inspection for safety-critical components (DigiQual)* is a collaboration between Imperial College (PI Peter Huthwaite) and University of Bristol funded by EPSRC and RCNDE. Imperial's work has been on the "bottom-up" task of making high-fidelity numerical simulations more efficient while the Bristol work has been "top-down" on making effective use of simulations for Inspection Qualification (IQ).

Purpose of this survey
As part of the Bristol work, we have published two papers that show how the classic *ahat-vs-a* approach to generate PoD curves can be generalised to cases where the standard assumptions cannot be satisfied [1] and how surrogate modelling and adaptive sampling can enable rapid visualisation of inspection performance for multiple parameters of interest [2]. The latter approach can be used as a tool to improve inspection design and also to identify worst-case scenarios, for example, to inform experimental test piece design. We have employed a Research Software Engineer to make these tools available as open-source software for industrial use to enable them to be trialled on real inspections. In broad terms, we envisage software that wraps around a user's preferred inspection simulation tool (e.g. a finite element package) that will:

1. provide a list of parameters for the inspection cases to simulate initially,
2. analyse the simulation outputs to produce, for example, PoD curves with quantified uncertainty, inspection performance visualisations,
3. provide a list of parameters for further cases to simulate to increase accuracy and reduce uncertainty.
4. the option to automatically iterate through (1-3) until a desired level of accuracy is obtained.

The anticipated software is likely to be offered in two forms: (a) a documented Python library that Python users can access directly, and (b) a graphical user interface that non-experts can use.

We are now at the point where we would like to get some input from potential users and would appreciate your input to whatever questions below you are able to answer. There are 13 questions and it should not take longer than 5minutes to complete.

The survey is anonymous unless you provide contact details in response to the final question.

References

[1] N. Malkiel, A. J. Croxford, and P. D. Wilcox, 'A generalized method for the reliability assessment of safety-critical inspection', *Proc. Roy. Soc. A*, vol. 481, no. 2312, 2025, doi: 10.1098/rspa.2024.0654.
[2] N. Malkiel, A. J. Croxford, and P. D. Wilcox, 'A comprehensive investigation of flexible and multi-dimensional simulation-based PoD analysis', *NDT and E International*, vol. 159, 2026, doi: 10.1016/j.ndteint.2025.103596.

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1. Your sector (tick all that apply)

- [ ] Aerospace
- [ ] Non-nuclear power generation

Summary

https://forms.office.com/e/pFDGgqpuJ8

https://pypi.org/project/digiqual

- 3D direct numerical simulation via FE is increasingly viable – 1000s simulations can be run in a few days
- Generalisation of $\hat{a}$ vs. a approach
- Exploration of multi-dimensional parameter space
  - Better understanding of inspection
  - Identification of worst-case scenarios
  - Optimisation of inspection design

- Try the Python version of DigiQual software (under development)!