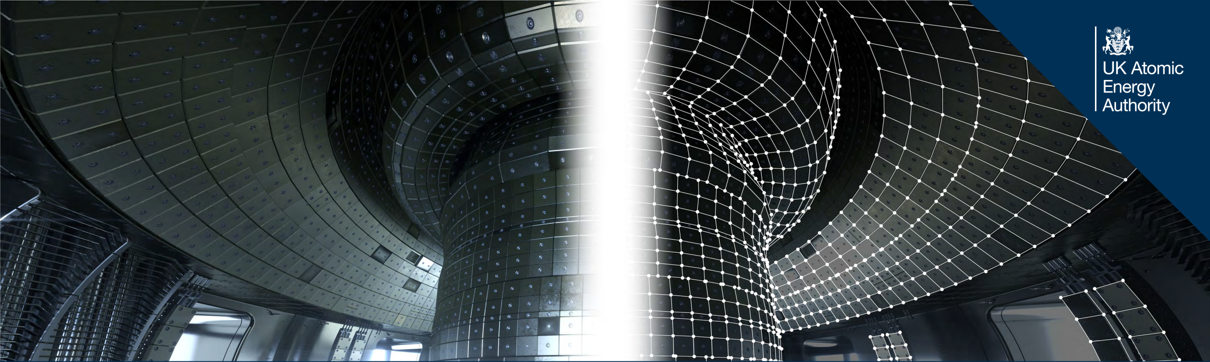

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Accelerating Breeder Blanket Design with Scalable Multi-physics Modelling and Digital Engineering Workflows

H. Brooks, L. Humphrey, S. Mungale, A. Davis, D. Mason, D. Foster | UKAEA

IAEA Technical Meeting on Tritium Breeding Blankets and Associated Neutronics
3 Sept 2025

Overview

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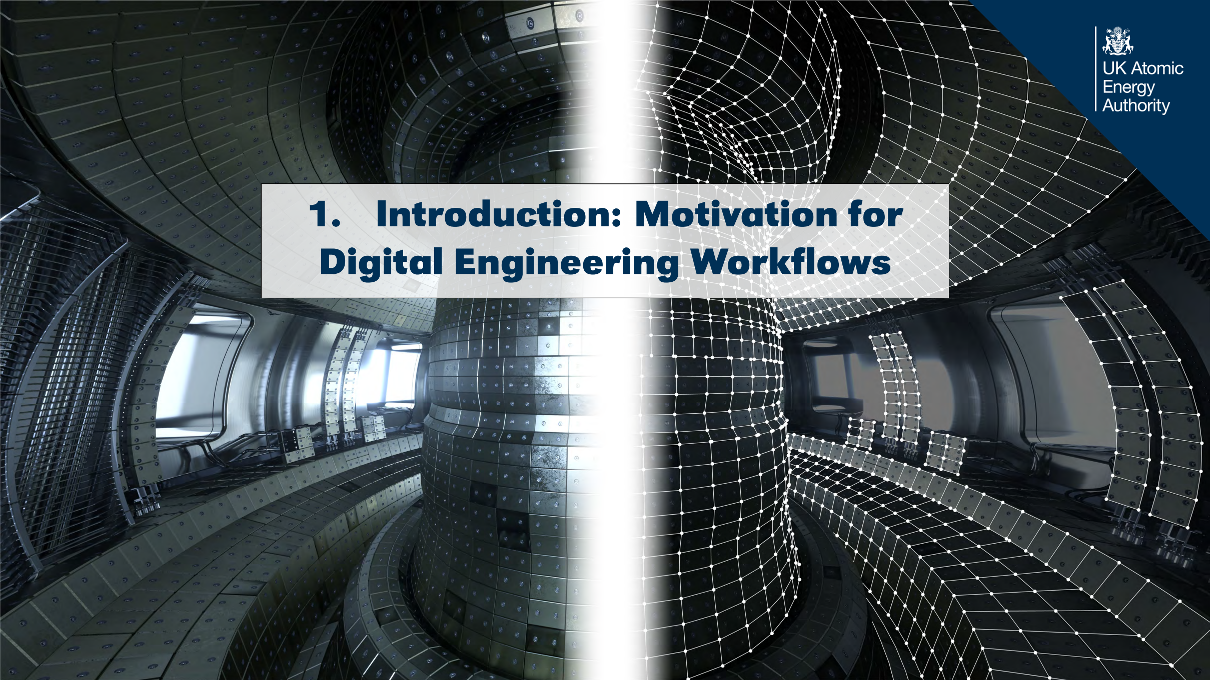
1. Introduction: Motivation for Digital Engineering Workflows
2. Tool-chain Overview
3. Geometric Optimisation of Solid Breeder Mock-up
4. Tritium Transport Sensitivity Study
5. Outlook and Summary

1. Introduction: Motivation for Digital Engineering Workflows



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Observations on the Design of Breeder Blankets

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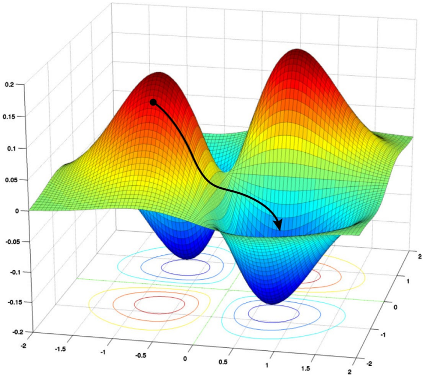
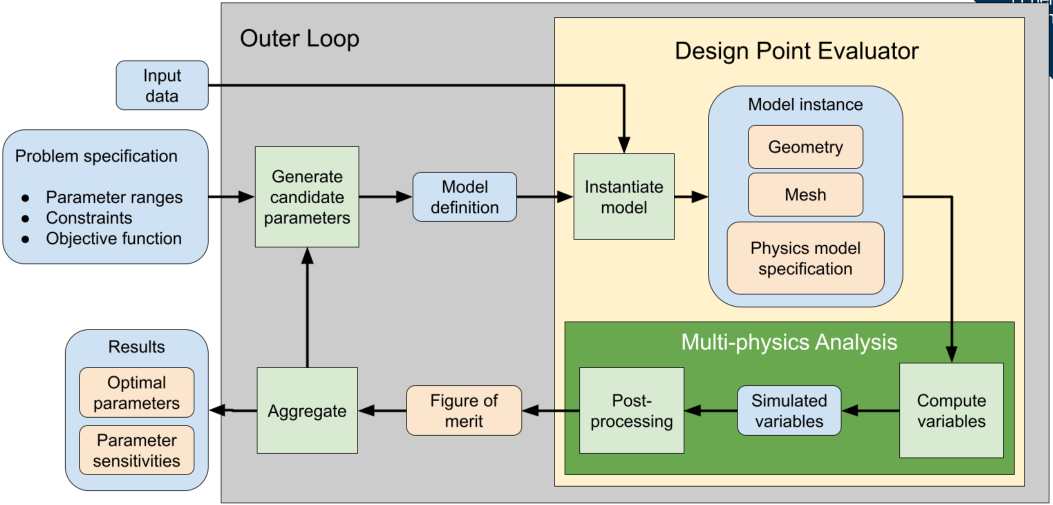
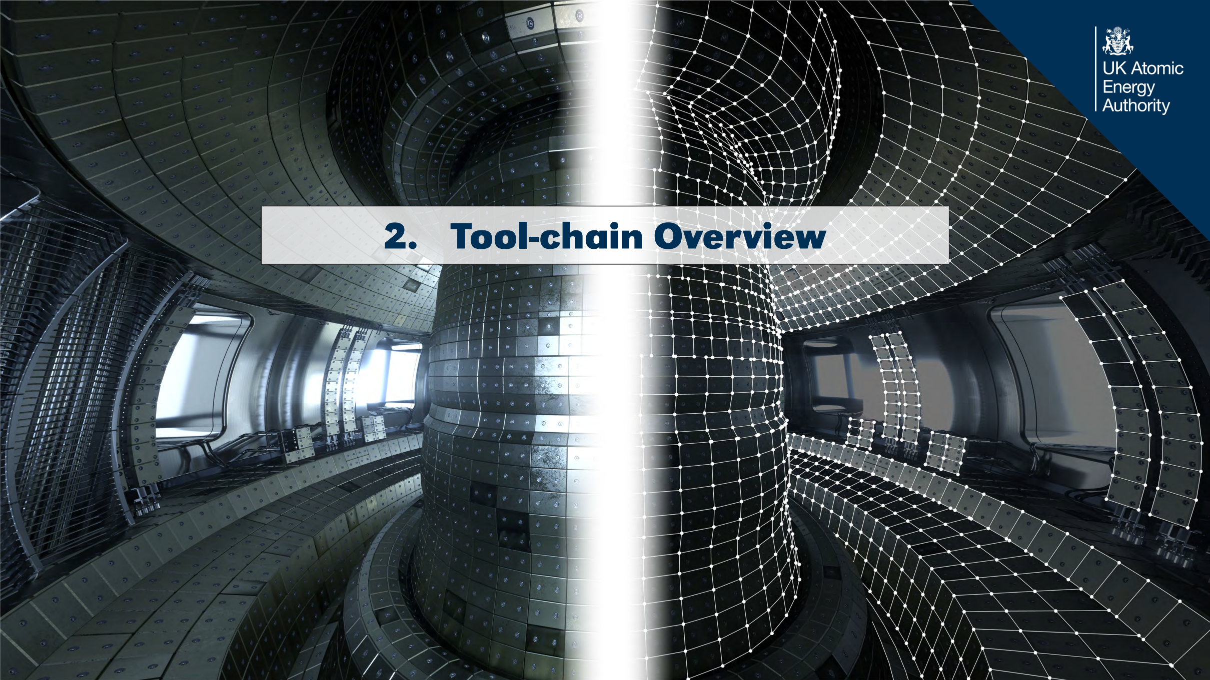
- Breeder blankets must satisfy many competing objectives and constraints
- Design space has a high dimensionality
- If overly conservative assumptions, risk incompatible constraints and null solution space
- Local optima may exhibit unituitive instabilities: risk rapid degradation of performance
- Brute force exploration of design space may not be feasible



Need to characterise the design space **holistically** and **efficiently**.

Idealised Digital Engineering Workflow





2. Tool-chain Overview

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SLEDO: A Sequential Learning Engineering Design Optimiser

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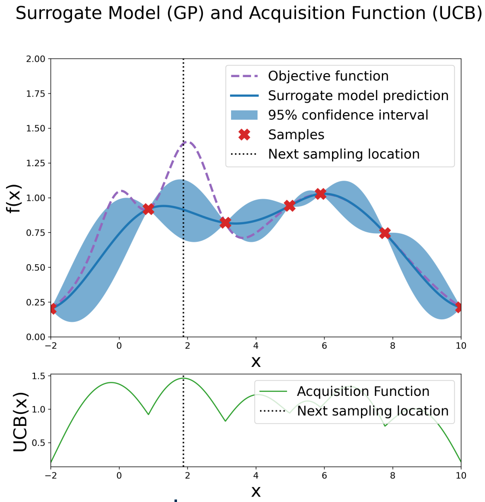

SLEDO performs Bayesian optimisation:

1. Given geometric parameterisation $\mathbf{x}$, define a search space and generate initial sample.
2. Train a **surrogate model** for the figure of merit $f(\mathbf{x})$: using a Gaussian Process regressor, obtain the mean and std deviation posterior $\mu(\mathbf{x})$ and $\sigma(\mathbf{x})$ for f.
3. Compute and maximise an **acquisition function** to generate subsequent trials, such as Upper Confidence Bound (UCB):

$$UCB(\mathbf{x}) = \underbrace{\mu(\mathbf{x})}_{\text{exploitation}} + \underbrace{\kappa\sigma(\mathbf{x})}_{\text{exploration}} \quad (1)$$

where κ is a tuneable hyperparameter.

Hypnos: Parametric Blanket Geometry Instantiator

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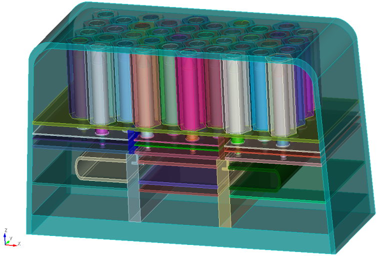
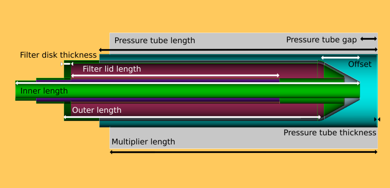
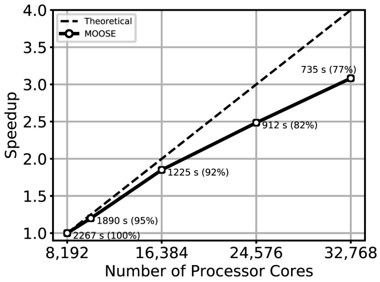
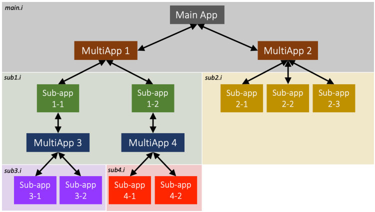




- Leverages Coreform Cubit **python API** to instantiate CAD from **geometric parameters**.
- Initial implementation focuses on Helium-Cooled Pebble Bed (HCPB) concept
- Hierarchical implementation of functional component classes: reflects **ontological relations** and increases **extensibility**
- Features: mesh generation, metadata (sideset, block, DAGMC material) assignment, metadata querying by component, material, interface
- Usable as command line **executable** or pip-installable **library**.

MOOSE for Multi-physics

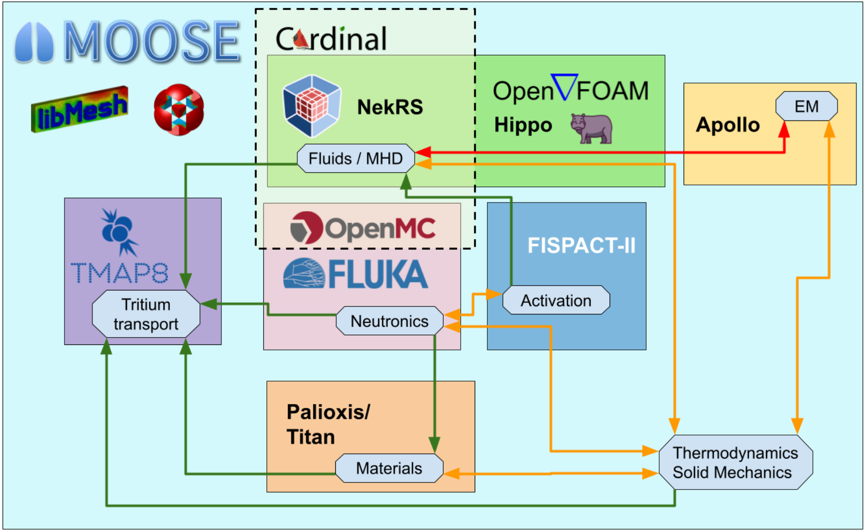




MOOSE is selected as a multi-physics platform:

- Proven scalability
- NQA1-compliant
- Good documentation and user support, active community
- Data structures which are conducive to tackling multi-physics, multi-scale problems, and wrapping external codes (e.g. `MultiApps`, `Transfers`)

Multi-physics Ecosystem



N.B. FISPACT-II and Fluka MOOSE applications are currently under development.

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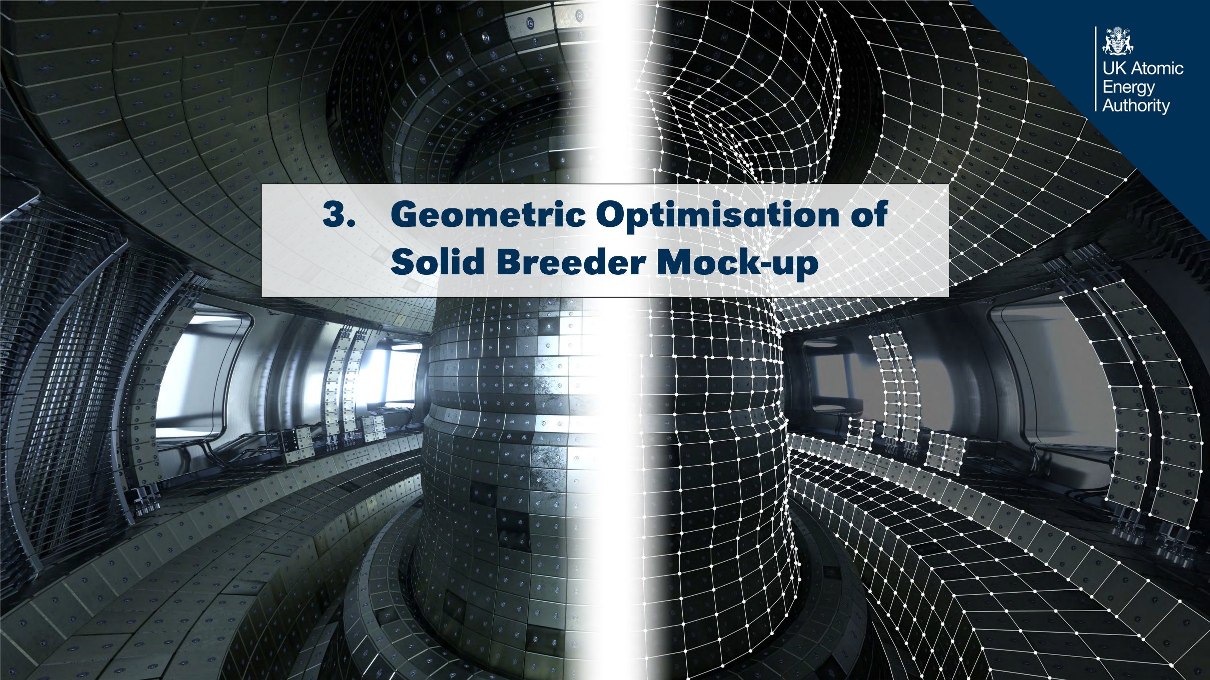
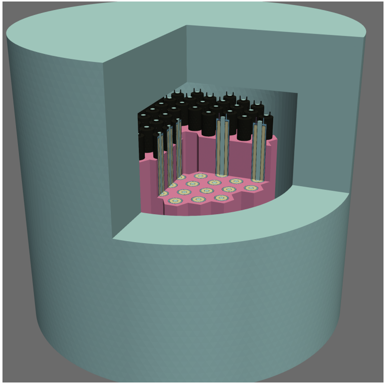


3. Geometric Optimisation of Solid Breeder Mock-up

LIBRTI Solid-Breeder Mock-up experiment



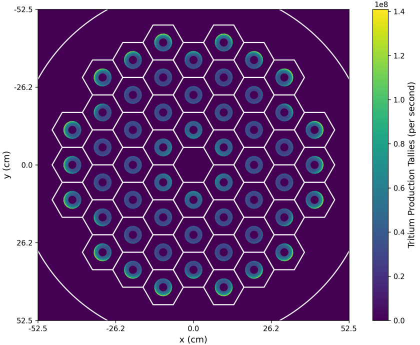
- **LIBRTI** (Lithium BReeding Tritium Innovation) is a UKAEA planned facility to test tritium breeding technology and validate modelling
  →See: Mark Gilbert's Talk, 15:00 Thu 4th Sept
- Compact 14 MeV neutron source
- Modular experimental set-up: here consider the solid-breeder concept (HCPB-like assembly of pins)
- Materials: KALOS breeder, steel cladding, helium coolant, lead multiplier, graphite reflector

Optimisation Analysis Setup

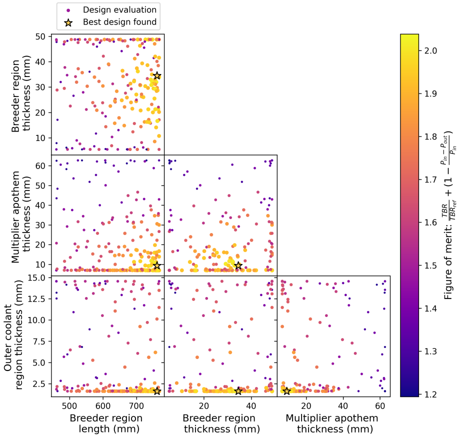
- Perform neutronics (OpenMC) and thermal hydraulics (MOOSE) analyses (not coupled)
- Figure of merit: weighted sum of TBR and pressure drop

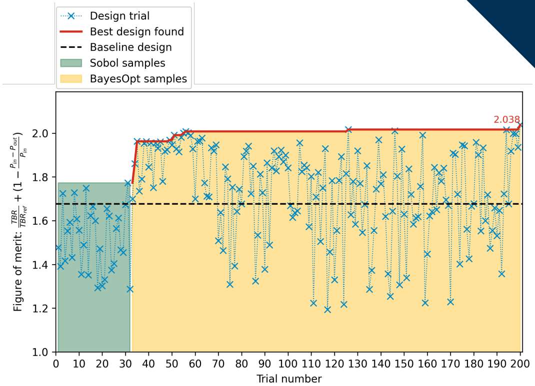
$$f = \frac{\mathrm{TBR}}{\mathrm{TBR}_{\mathrm{ref}}} + \left(1 - \frac{p_{in} - p_{out}}{p_{in}}\right)$$

- Vary: breeder / coolant / multiplier thicknesses, pin length. Number of pins is maximum to fit inside a fixed radius.
- Acquisition function: expected improvement
- Perform 200 trials, of which 32 Sobols samples

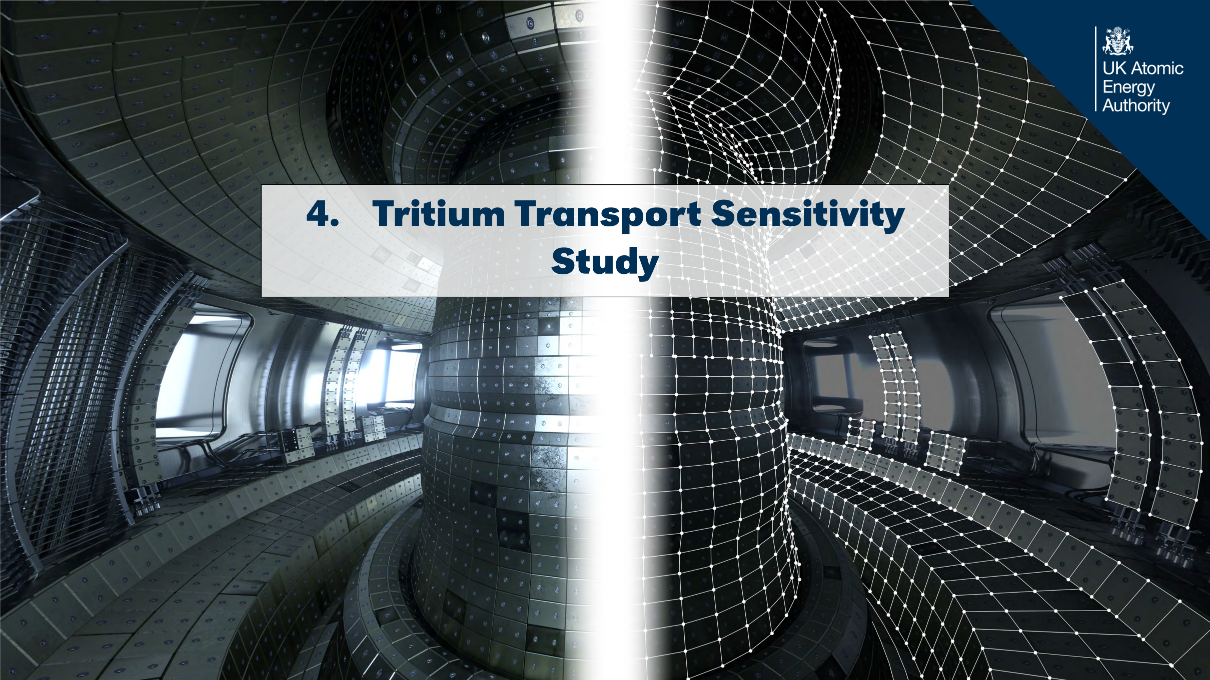


Optimisation Results





4. Tritium Transport Sensitivity Study



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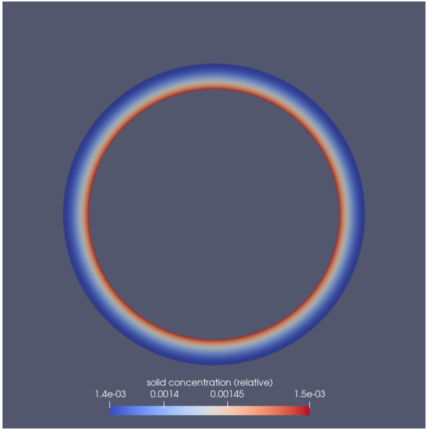
UQ Analysis Set-up



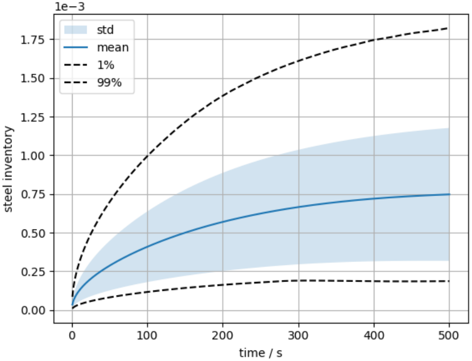
- An optimized design means little if it is not **robust** to perturbations.
- We also need to perform **uncertainty quantification**
- Major source of uncertainties is tritium permeation: perform sensitivity study to transport parameters (at constant temperature)
- TMAP8 Model: diffusion of single species from porous breeder region (diatomic) into steel (monoatomic), with Sievert's Law applied at the interface as a constraint:

$$c_s = K_0 \exp\left(\frac{-E_K}{RT}\right)\sqrt{c_g RT}$$

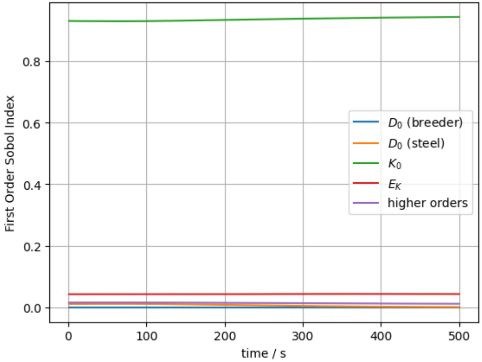
- Vary: K_0, E_K, D_0 by $\pm 20\%$

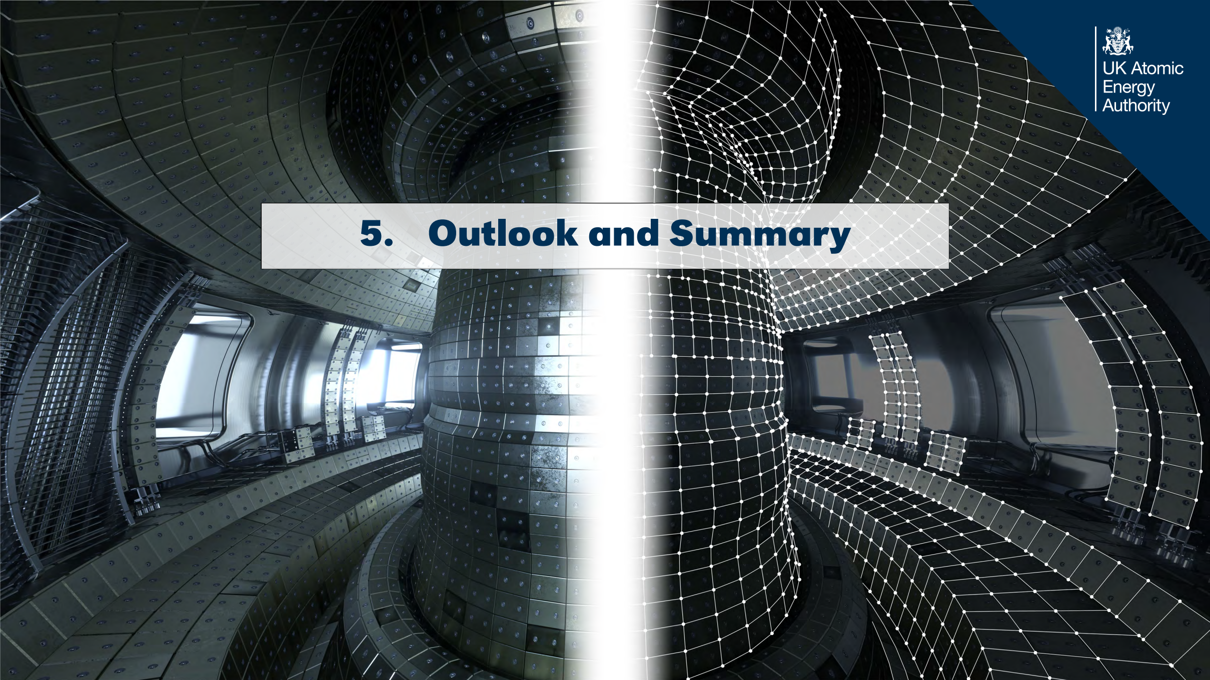
UQ Results

Uncertainty (standard deviation) is 60% on last timestep.



Highest sensitivity is to K_0, followed by E_K.





5. Outlook and Summary

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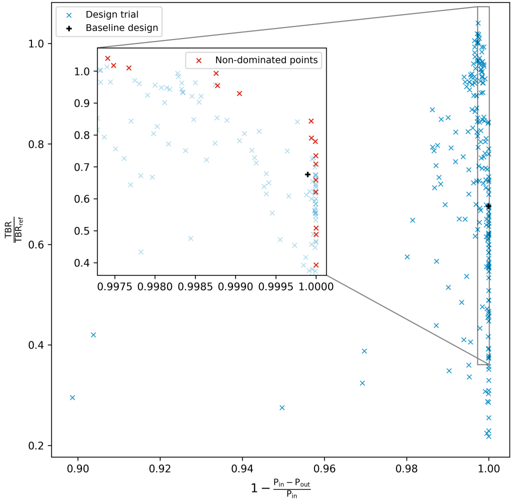
Outlook: Optimisation Improvements



Initial parametric geometry optimisation was intended to demonstrate the methodology. A more thorough analysis should include:

- Multi-objective optimisation: sampling of pareto front
- Coupling of multi-physics: neutronics, thermal, fluids, tritium transport...
- Include more performance indicators: e.g. uncertainty, cost

Outlook: Tritium Transport Modelling

Tritium transport sensitivity study was overly simplistic; modelling should include:

- Minimally: multiple hydrogen isotopes, trapping, isotopic exchange, speciation
- Ideally: multi-scale treatment for retention and permeation (with a surrogate for microscale physics?)

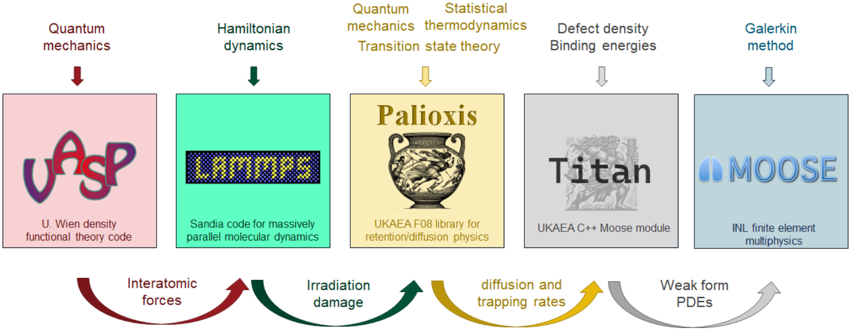


Image courtesy of Daniel Mason. See also: Kaur et al "The effect of multi-occupancy traps on the diffusion and retention of multiple hydrogen isotopes in irradiated tungsten and vanadium" [arXiv:2508.15341]

Summary

- We have developed a scalable digital engineering pipeline for breeder blanket design consisting of:
  - **SLEDO:** design space exploration and Bayesian optimisation
  - **Hypnos:** parametric blanket geometry instantiator
  - **MOOSE:** flexible multi-physics analysis
- Bayesian methods can be effective at characterising the behaviour of a given figure of merit within a multi-dimensional parameter space space and **improving the design.**
- Combined with UQ, this will permit assessment of **robustness** and **design of experiments.**

See also:

- github.com/aurora-multiphysics/sledo
- github.com/aurora-multiphysics/hypnos
- github.com/idaholab/moose