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Machine Learning Techniques for Sequential Learning Engineering Design Optimisation

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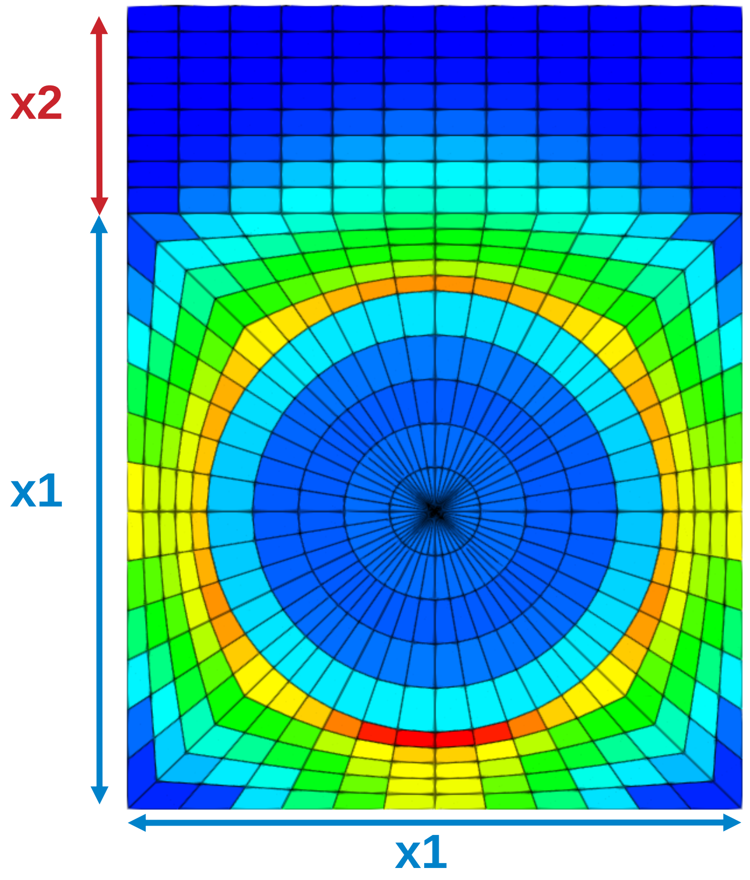
Introduction

- To **optimise** an **engineering design:**
  1. **Describe** the **design parametrically**.
  2. **Select** an/some **optimisation metric(s)**.
  3. **Seek** the **value(s)** of your chosen **parameter(s)** which optimise your chosen **metric(s).**
- **Machine learning (ML)** can **intelligently select next candidates** during an **optimisation sequence**.
- This allows us to make **best use of HPC resources: reducing** the number of **expensive-to-evaluate HPC simulations** required to optimise the design.
- However, the engineer must select appropriate:
  - **Parameters to vary** and their **bounds.**
  - **Optimisation criteria** and their **weights.**
  - **Choice of ML technique to suit the problem.**



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In this talk...

Sequential Learning Engineering Design Optimisation

- Surrogate models & acquisition functions.
- Bayesian optimisation.
- Example: optimising a 2D Test Function.

Simple Divertor Monoblock Model

- Context for the model (HIVE Experiments).
- Building the model in MOOSE.
- Optimising the model in BoTorch.

Next steps

- Increasing model complexity.
- Improving the surrogate model.
- Exploring machine learning techniques.

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Surrogate Models & Acquistion Functions

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Surrogate models are statistical models trained on a dataset used to interpolate between expensive-to-evaluate data.

e.g. a *gaussian processor (GP)*

Acquisition functions are cheap-to-evaluate functions used as a loss-function when training surrogate models.

e.g. *expected improvement (EI)*

exploitation term **exploration term**

$$EI(x) = \begin{cases} \boxed{[\mu(x) - f(x^+) - \xi]\Phi(Z)} + \boxed{\sigma(x)\varphi(Z)} & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0 \end{cases}$$

$$Z = \begin{cases} [\mu(x) - f(x^+) - \xi]/\sigma(x) & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0 \end{cases}$$

$\mu(x)$: mean posterior $\sigma(x)$: std posterior

x^+: best point so far $f(x^+)$: best value so far

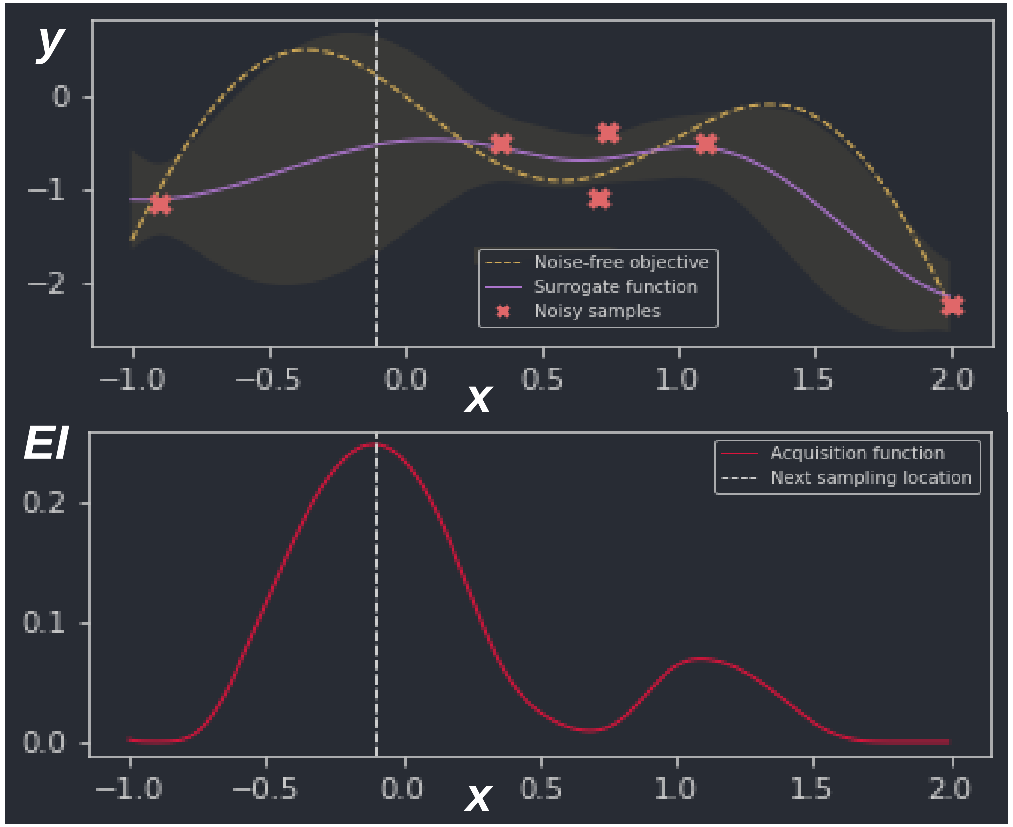
Φ, φ: CDF and PDF of normal distribution

ξ: exploration parameter (default = 0.01)

Key takeaway: **exploitation** vs **exploration**

Above: GP model trained on noisy samples for a simple 1D function: $\boldsymbol{y = -\sin(3x) - x^2 + 0.7x}$

Below: EI for the model, indicating the best location to sample next.



Bayesian Optimisation

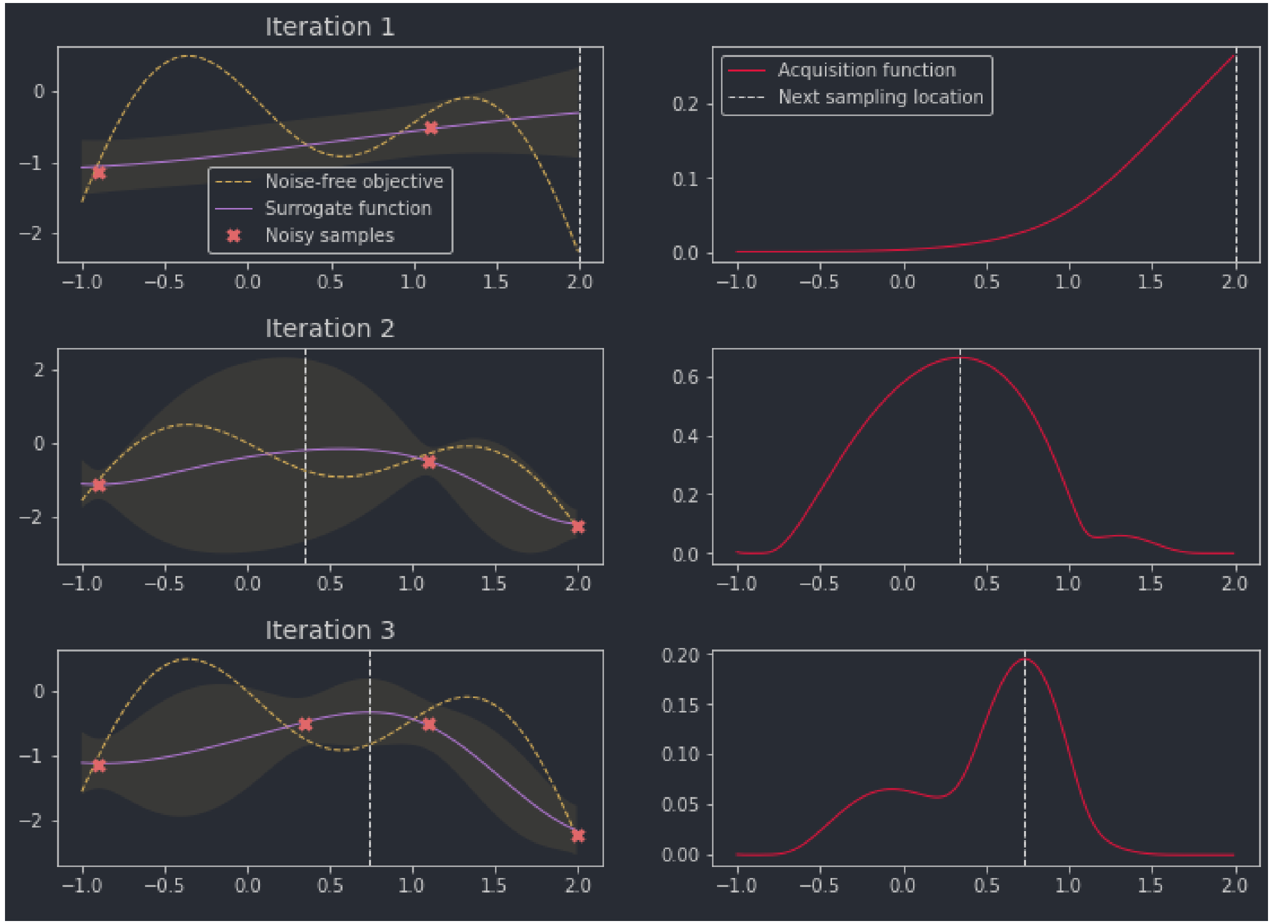
*"**Sequential design** strategy for **global optimisation** of a **black-box function**."*

- **Goal is finding optimal design,**
  training the surrogate is a means to that end but not the goal.
- **Black-box is the HPC Simulation,**
  inputs = simulation parameters
  outputs = optimisation criteria

BayesOpt loop:

1. **Train surrogate model** on initial simulations.
2. While **acquisition f^n > some threshold**:
   i. **Optimise acquisition function** to find the best candidate to simulate next.
   ii. **Evaluate** that point with a **HPC simulation.**
   iii. **Retrain model** and repeat.

Simple 1D example.



Bayesian Optimisation:
2D Test Function

PyTorch
BoTorch

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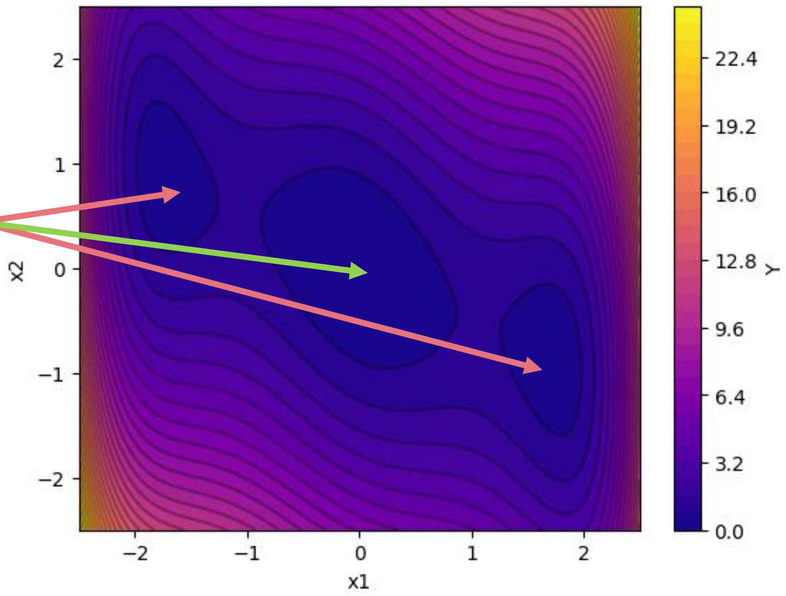
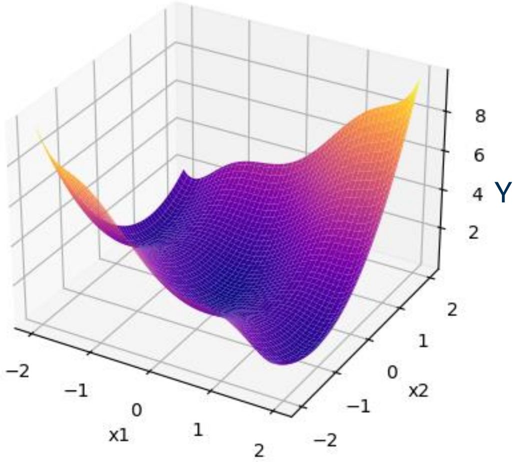
Three Hump Camel

Seeking global minimum at (0, 0).

Three local minima.

i.e. must find the goal while avoiding two traps.

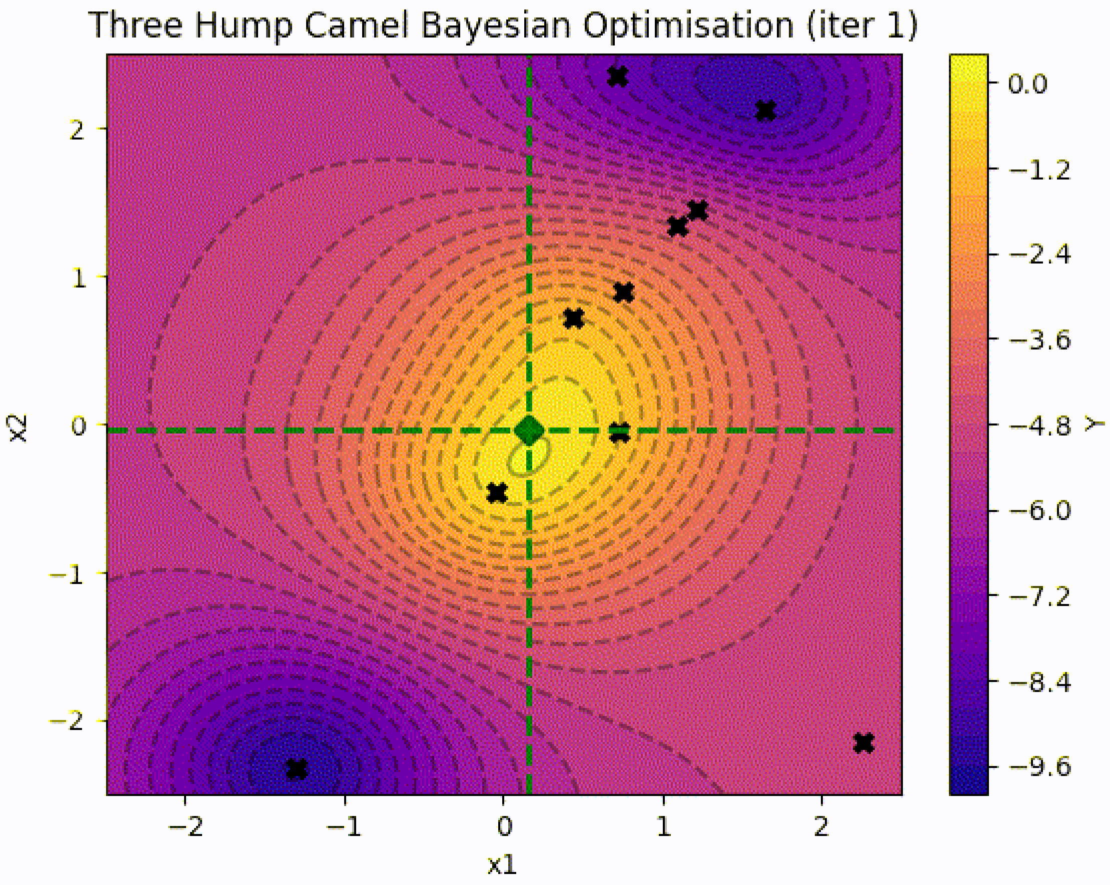





```
X={x1, x2} 2D inputs
Y          1D output
```

Bayesian Optimisation Loop

(note: **Y** inverted to seek $\mathbf{Y_{min}}$ by maximising **-Y**)



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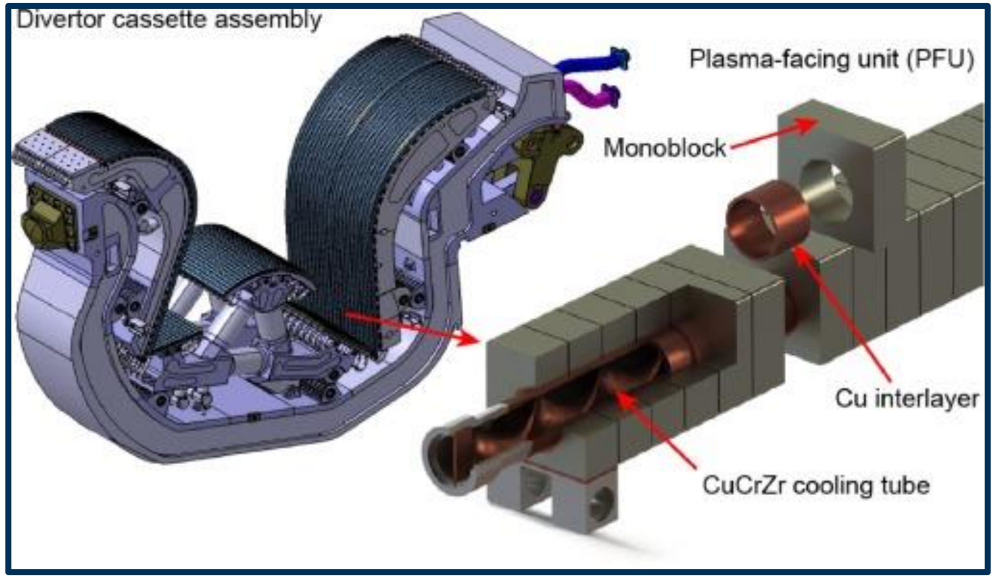
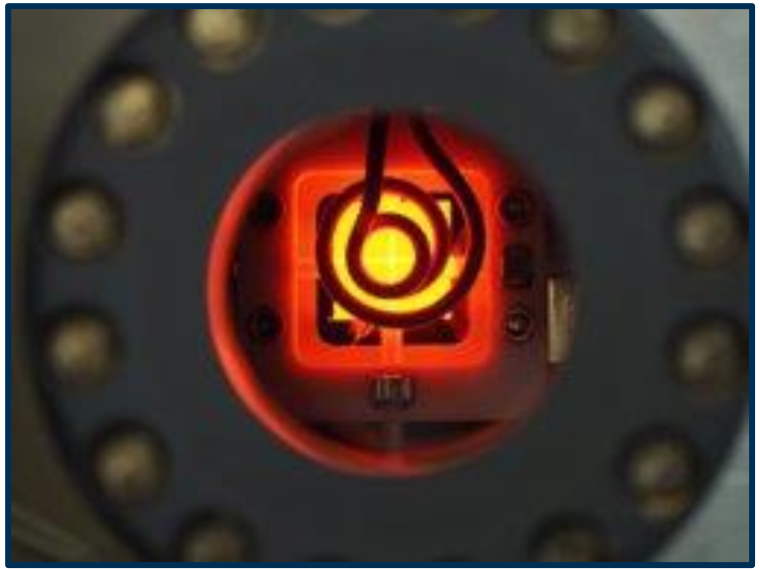
Simplified Divertor Monoblock Model

- A **divertor monoblock** is a modular cooling component used in tokamak divertors.
- A **simplified model** containing a **filled interlayer** will be tested in **HIVE**; this makes an ideal **low-parameter component** for a **proof-of-concept optimisation**.



Monoblock detail within a tokamak divertor.
Image source: Pitts et al. (2017)



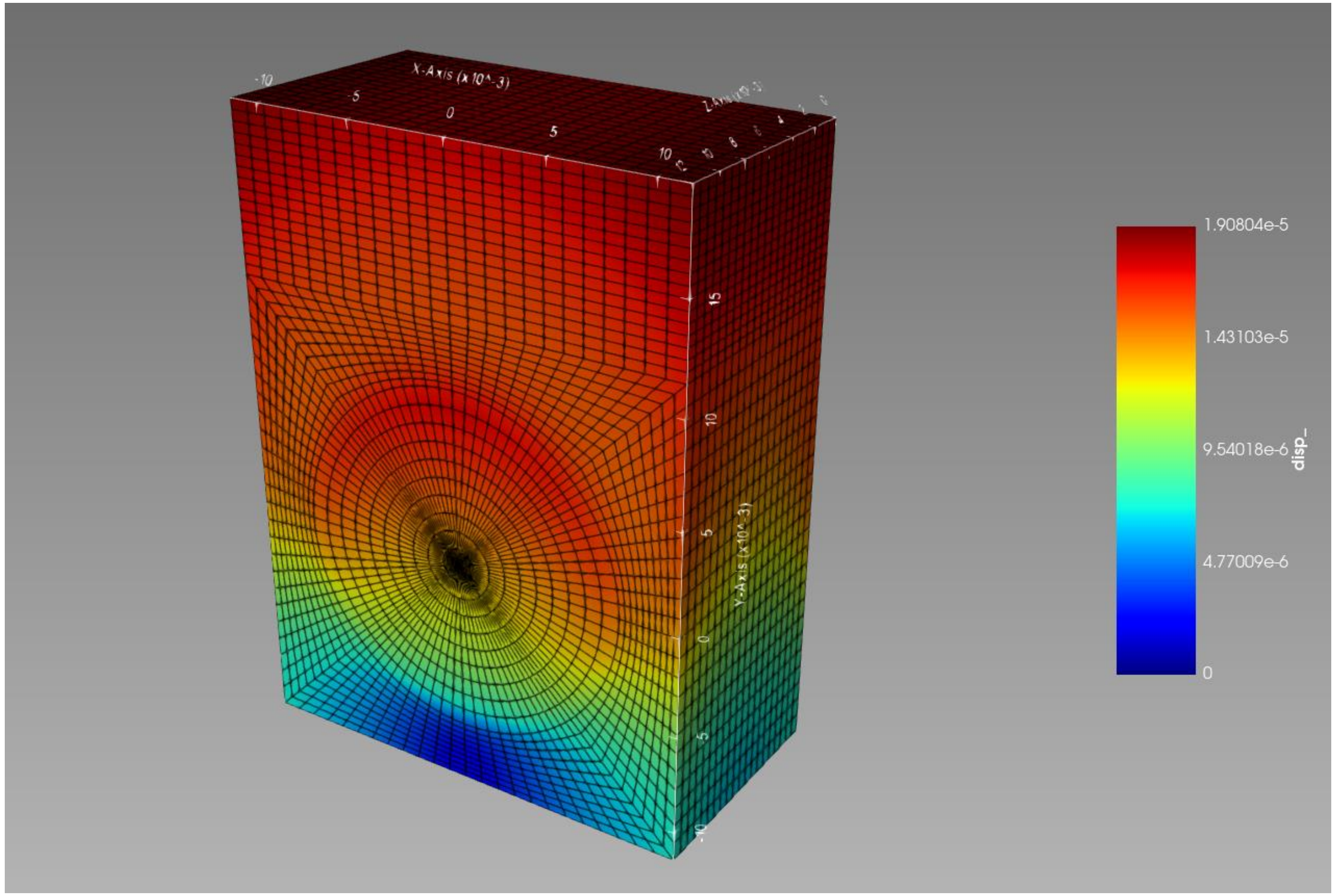
HIVE testing facility.
Image source: CCFE website

Simple monoblock physical model.
Photos by: Adel Tayeb, UKAEA

Simplified Divertor Monoblock Model

MOOSE

- **Steady state thermomechanical** solution.
- **Parametric** geometry & meshing.
- **Stress-free temp 20°C.**
- **Uniform temp 100°C.**
- Model **pinned at base,** allowed to deform elsewhere.



Displacement magnitude field.

Simplified Divertor Monoblock Model

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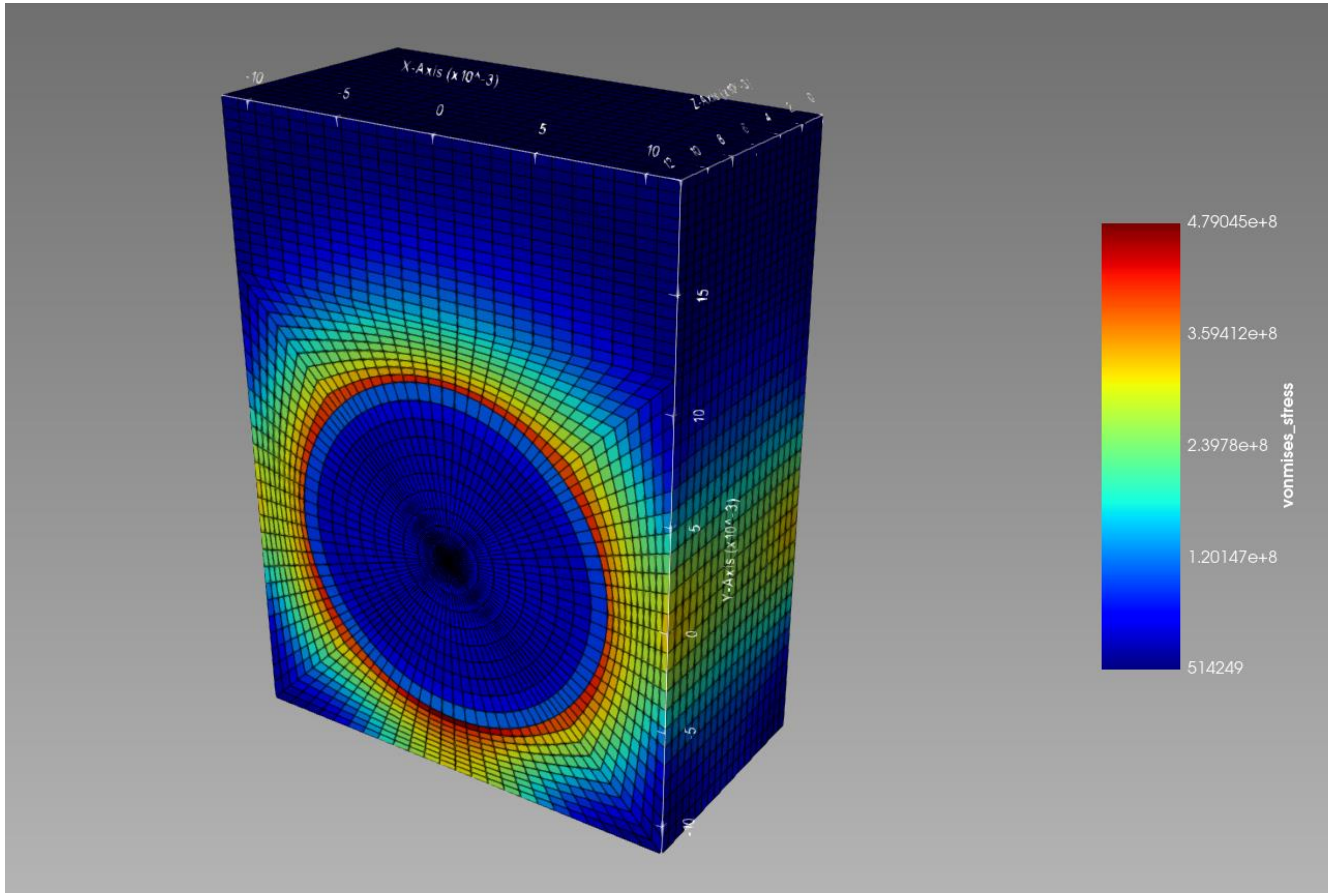
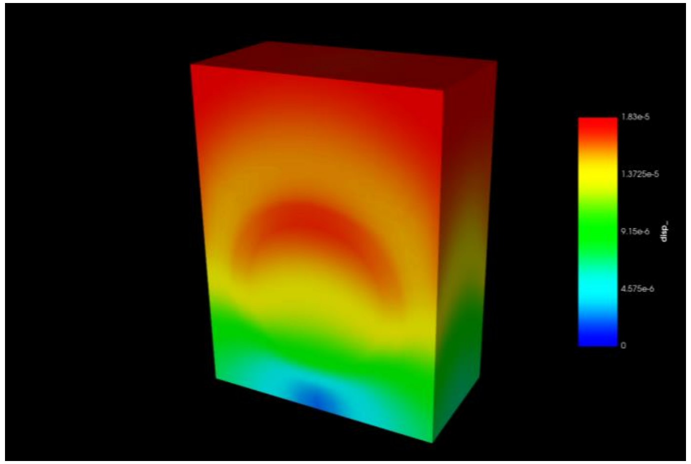


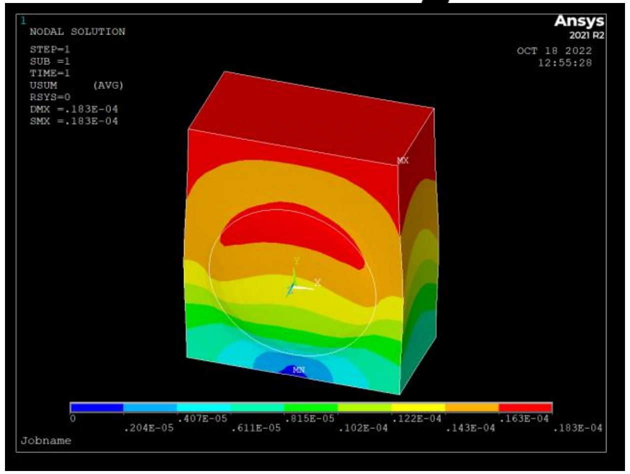
Thermal expansion (Von Mises) stress field.

Simplified Divertor Monoblock Model

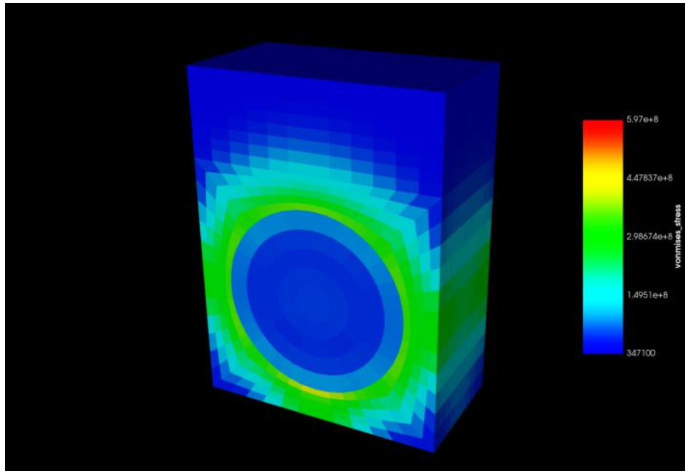
MOOSE | Ansys

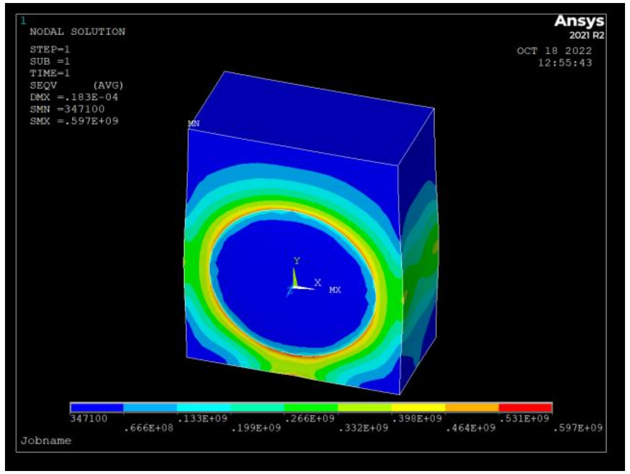
Displacement Magnitude





Thermal Stress





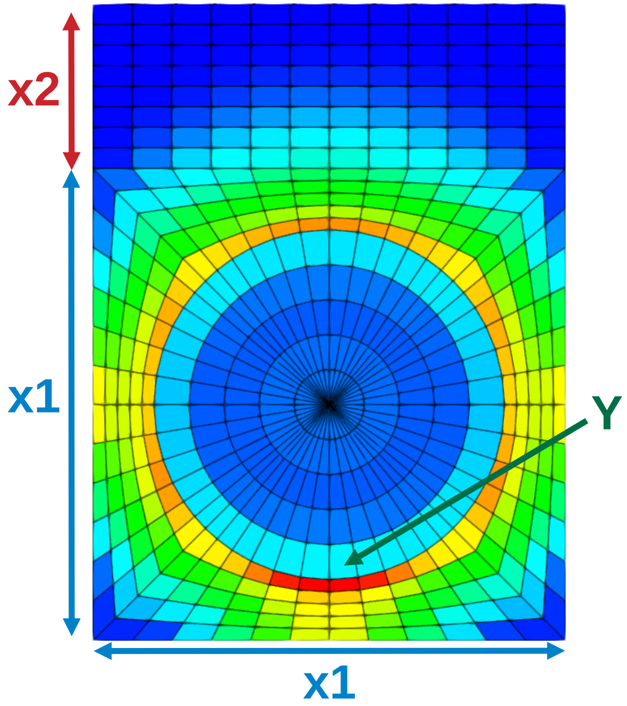
Validation of results against Ansys models.

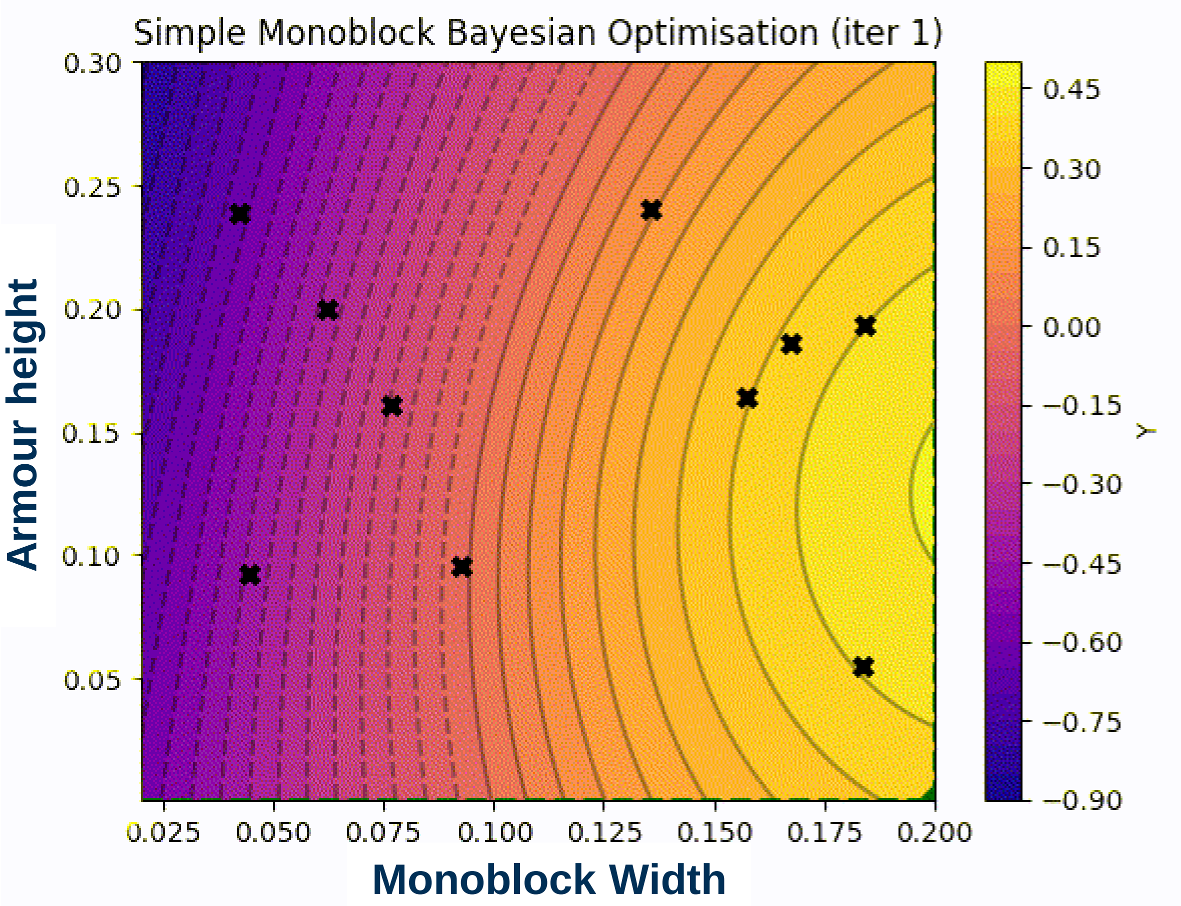
Ansys models by: Lloyd Fletcher, UKAEA

Optimising the Model

Using the same GP + EI model as before, with the following chosen parameters:

- x1 = monoblock width
- x2 = armour height
- Y = maximum thermal stress





Optimising the Model: Results

Optimal design found at:

width = 83 mm,
armour height = 1 mm

Compared to original settings:

width = 23 mm,
armour height = 8 mm

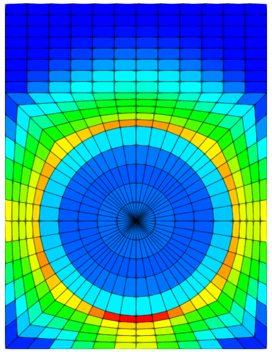
Issues:

- **Only stress is considered.**

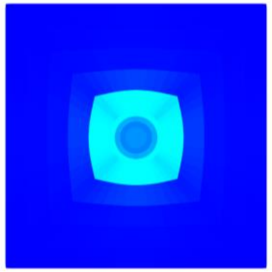
  A **full physics model** should be **multi-objective:** also minimising the required pumping power to maintain operational temperatures.

- **Too few parameters.**

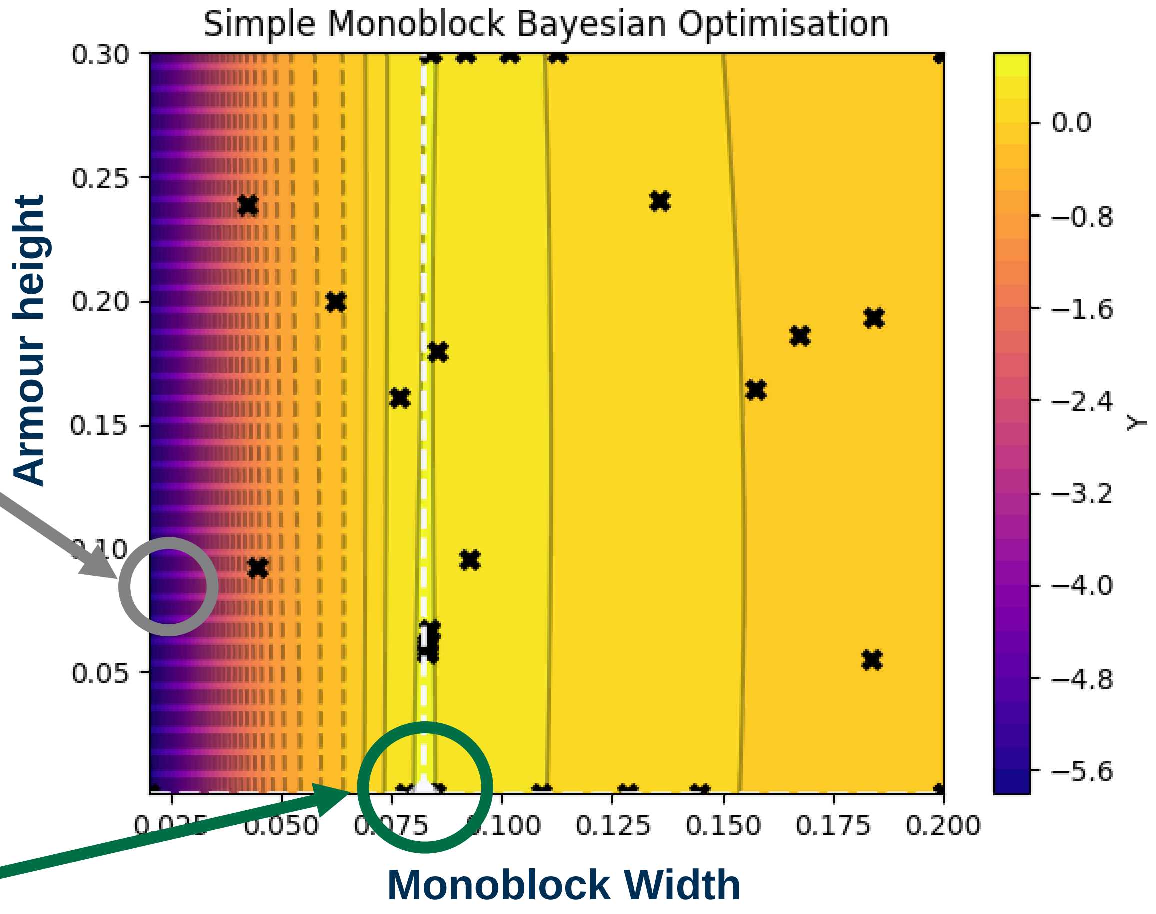
  Creates a non-representative design space for fusion problems. A **full physics model** will produce a **higher dimensional design space**.



Original design



Optimised design



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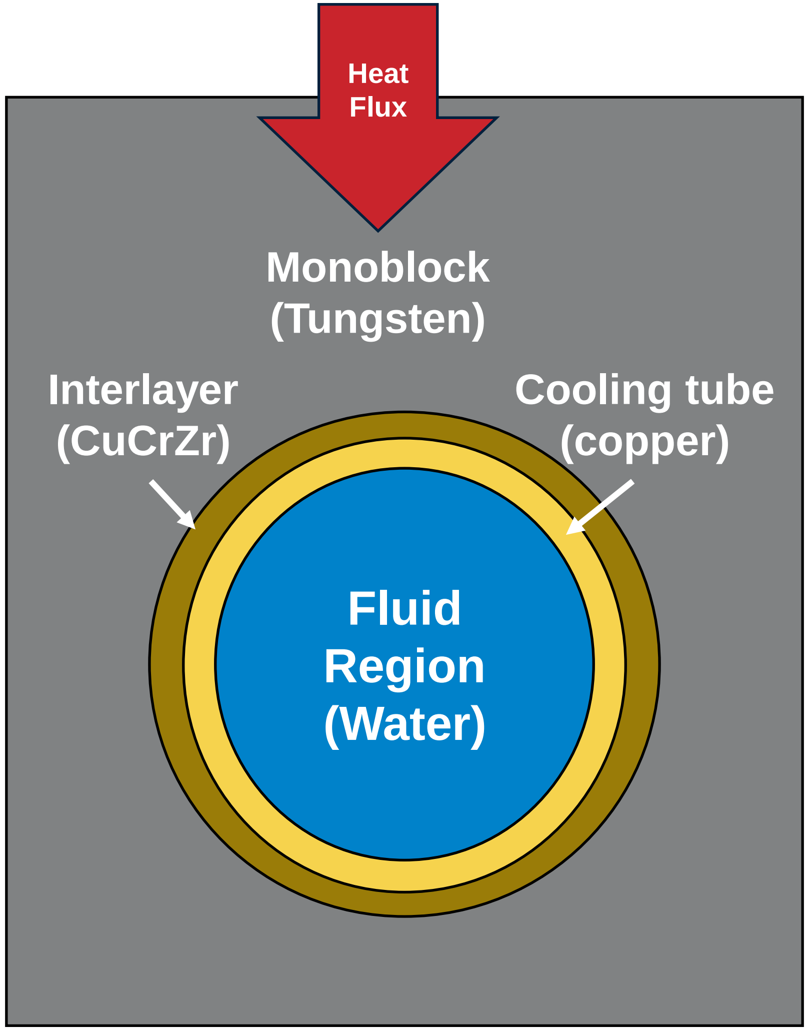
Next Steps: Model Complexity

1. **Intermediate complexity model:**
   1. Add **copper pipe**, bringing $\mathbf{n_{dim} = 6}$.
   2. Add **directional heat flux** on the armour.
   3. Add **cooling** as **convection flux** on pipe.
2. **Full Physics model:**
   1. Add **non-linear materials** including plasticity & visco-plasticity.
   2. Add **cooling** as **coupled CFD** (computational fluid dynamics).
   3. Run **transient simulation** with full thermal history (manufacturing phase & thermal pulses during operational phase in a tokamak).



Basic schematic of full physics model

Next Steps: Surrogate Modelling

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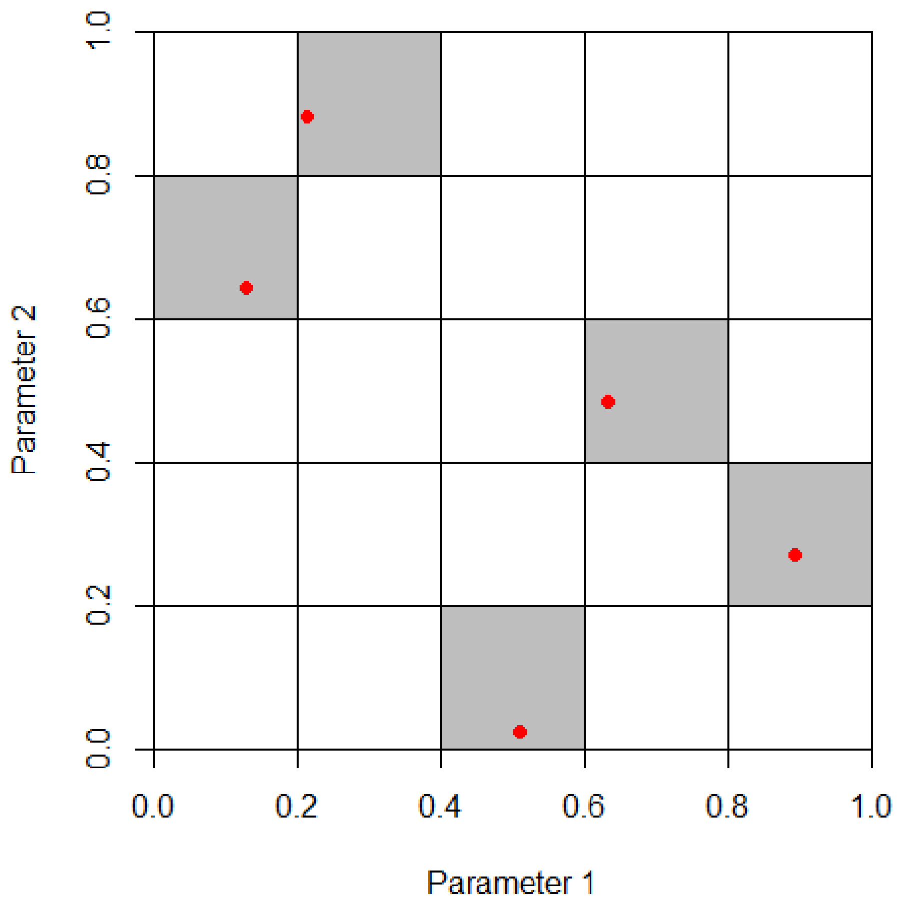
1. **Run multi-objective optimisation:**
   i. Avoid maximum temperature exceeding operational limits. Note: this is a **non-linear step discontinuity**.
   ii. **Minimise pumping power in CFD** on full physics model.
2. **Improve sample plan:**
   i. **Initial samples** were **selected randomly** from a **uniform distribution** within the bounds. Using a rule of thumb: **10 x ndim = 20 points**.
   ii. A **more sophisticated sample plan** (e.g. Latin Hypercube) would **improve the initial surrogate model**.



2D Latin Hypercube with 5 points

Next Steps: Exploring ML Techniques

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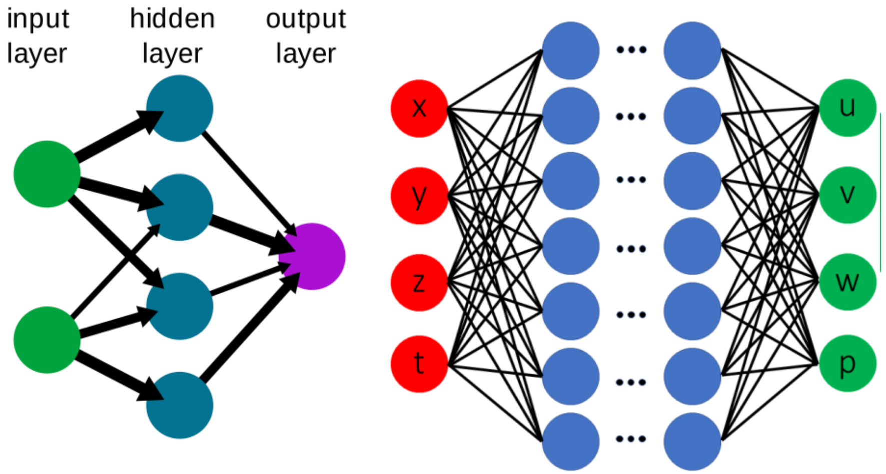
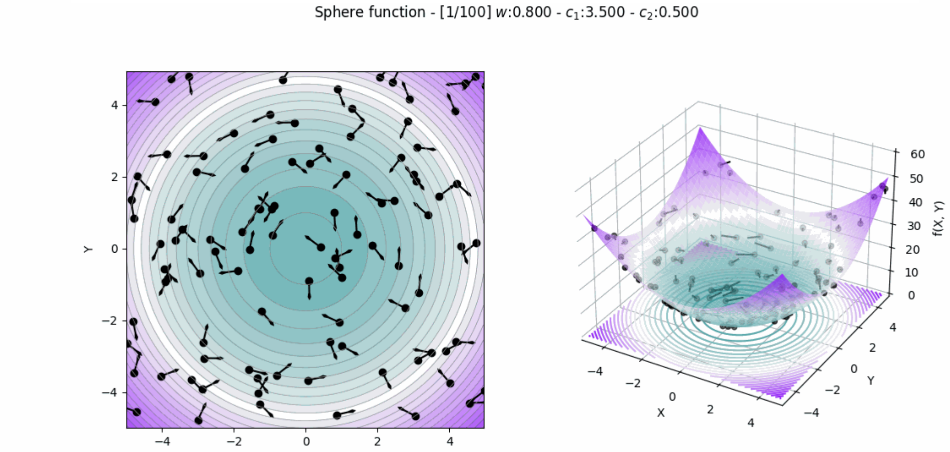
- **Neural network (NN)**
  - **strength:** identifying non-linear patterns in design space
  - **challenge:** lack of well-defined acquisition functions
- **Physics-informed neural network (PINN)**
  - **strength:** encoding known physics to train well on small datasets
  - **challenge:** lack of well-defined acquisition functions
- **Particle swarm optimisation**
  - **strength:** parallel optimisation, built-in exploration
  - **challenge:** potential overuse of HPC simulations as the model is updated after multiple parallel simulations



Left: **Simple NN**, Right: **PINN**

Images from: Wikipedia



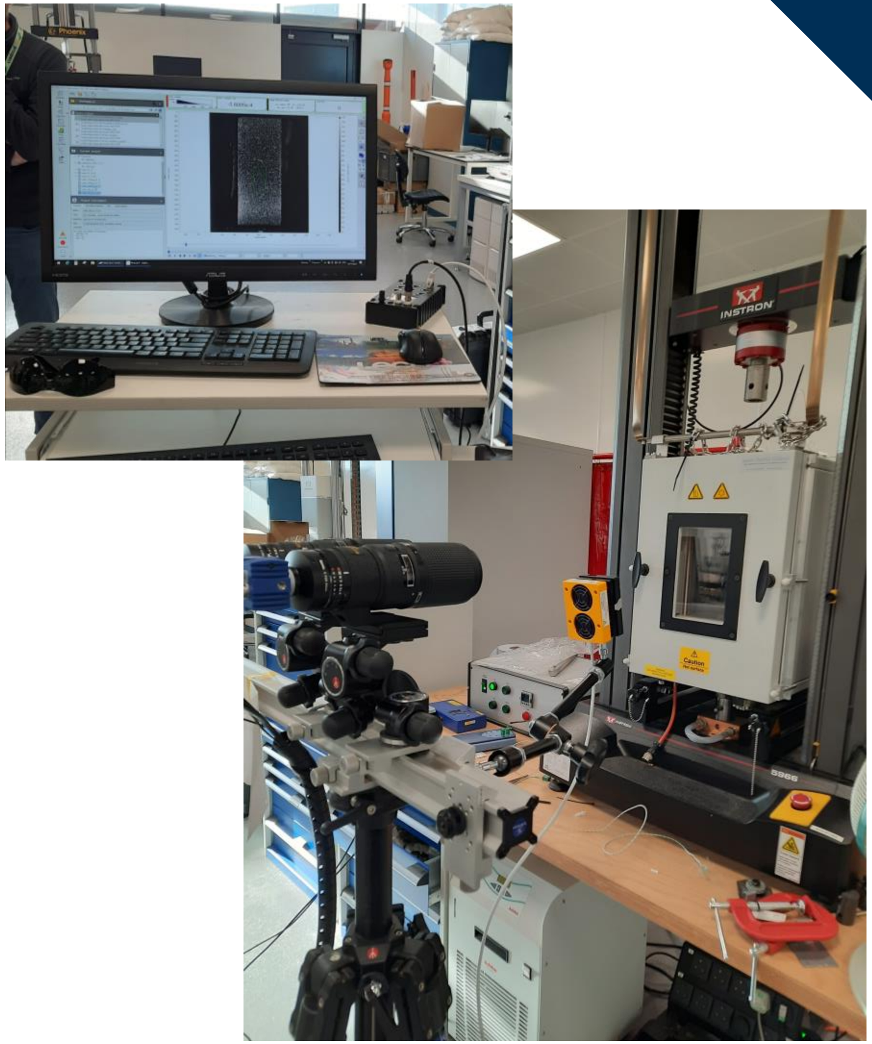
Particle swarm optimisation

Visualisation by: Axel Thevenot, Towards Data Science

Related Projects

- **Machine Learning for Component Validation**
  - A summer student placement project to utilise **ML methods** for data validation of **HIVE monoblock experiments**.
  - Project will use the **MOOSE monoblock** models generated in this project.

- **Proteus Development**
  - **Proteus** is a **MOOSE app** focussed on **coupled fluid dynamics**, developed as part of the **Aurora multiphysics package**.
  - The **monoblock simulations** are being contributed to **Proteus** as **example thermomechanical problems**.



Stereo digital image correlation (DIC) setup gathering thermal stress data from the simple monoblock model.

Photos by: Adel Tayeb, UKAEA

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Acknowledgements

For an introduction to surrogate modelling and general support throughout the project.

- **Aleksander Dubas**, UKAEA

For advice on modelling the monoblock and providing the Ansys models:

- **Lloyd Fletcher**, UKAEA

For advice on ML concepts and support with BoTorch:

- **Lorenzo Zanisi**, UKAEA
- **William Hornsby**, UKAEA
- **Timothy Nunn**, UKAEA

Software used:

- MOOSE **https://mooseframework.inl.gov/index.html**
- Aurora Multiphysics / Proteus **https://github.com/aurora-multiphysics/proteus**
- Scikit-learn **https://scikit-learn.org/stable/**
- PyTorch **https://pytorch.org/**
- GPyTorch **https://gpytorch.ai/**
- BoTorch **https://botorch.org/**
- Matplotlib **https://matplotlib.org/**

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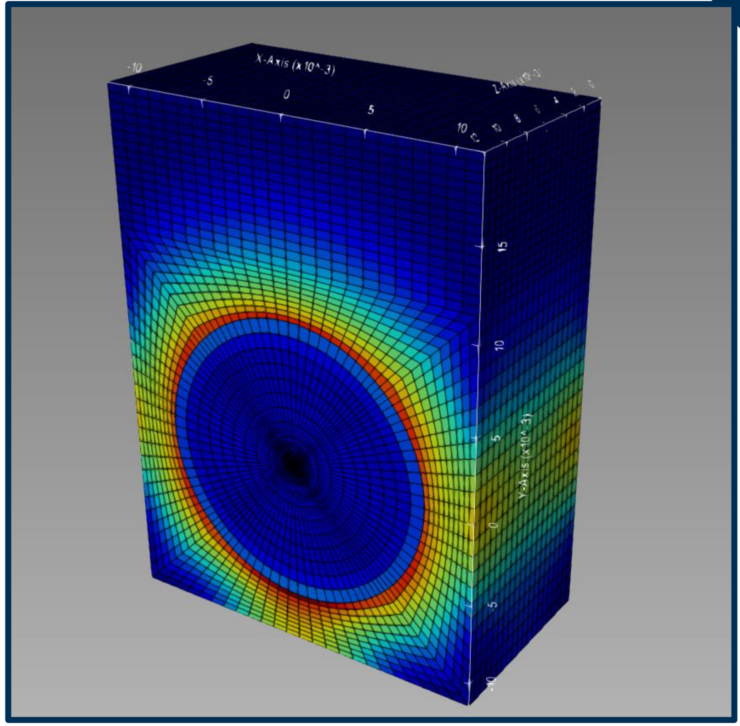
Summary

- **ML** allows us to make **best use of HPC** resources in **sequential learning engineering design optimisation.**
- **Proof of concept Bayesian optimisation** of a **simple divertor monoblock.**
- **Next steps** towards a **range of optimisation techniques** on **multiple levels of complexity.**



Please feel free to contact me with questions, feedback, and suggestions!

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