Uncertainty Quantification and Reliability of Fusion Materials

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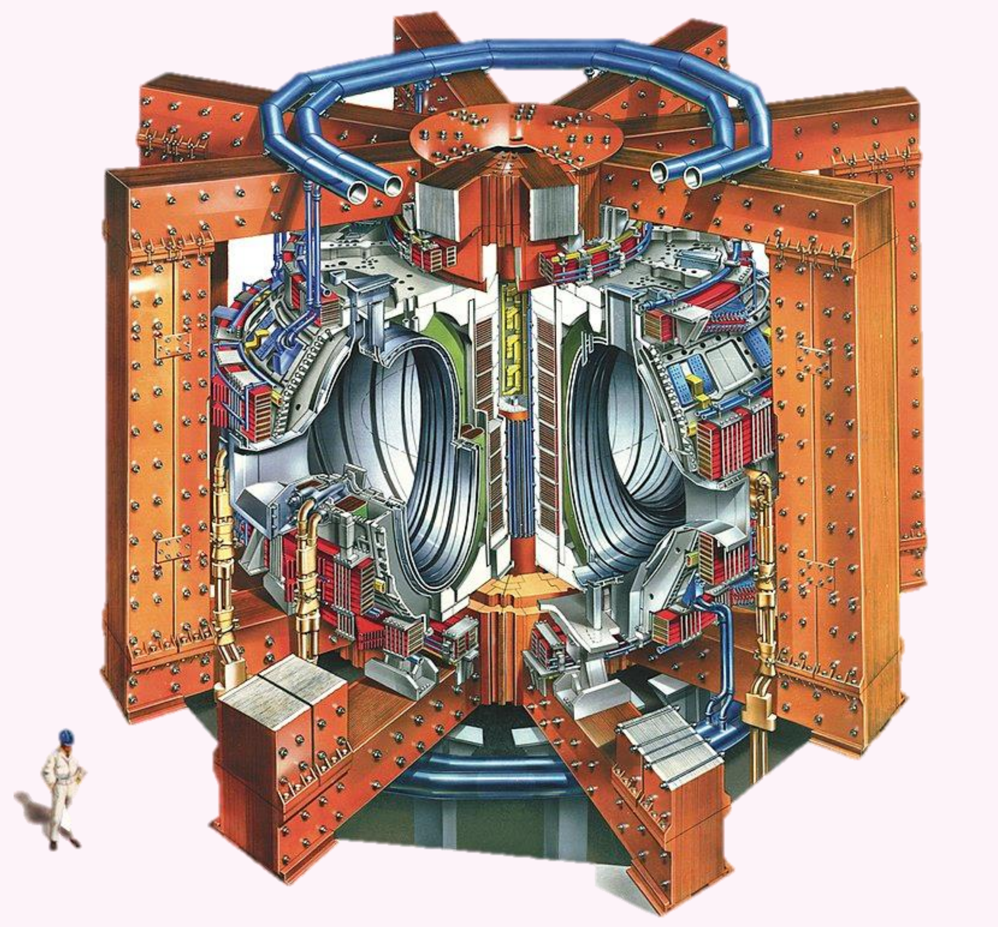
Introduction

- The development of plasma-facing materials able to withstand the extreme conditions inside a tokamak reactor is crucial for achieving nuclear fusion.
- Assessing risk of failure and uncertainty quantification in material behaviour is urgently needed to accelerate design and qualification of reactor components.
- This investigation focuses on comparing uncertainty quantification methods for rare event simulations of material failure. We compare the results of direct Monte Carlo simulations with an iterative subset method.
- The results of this investigation will be used to inform the choice of uncertainty quantification algorithms at the UKAEA in future materials qualification exercises for first-wall plasma facing materials.

Fusion Reactors

- The Joint European Torus (JET), built in 1983 was able to produce the first controlled plasmas and in 1997 produced an energy gain factor of 0.65 [1]. This was only recently bested by the National Ignition Facility who reached an energy gain factor of 1.54 with a 3.15 MJ output from a 2.05 MJ input [2].



Modelling of Crystal Plasticity

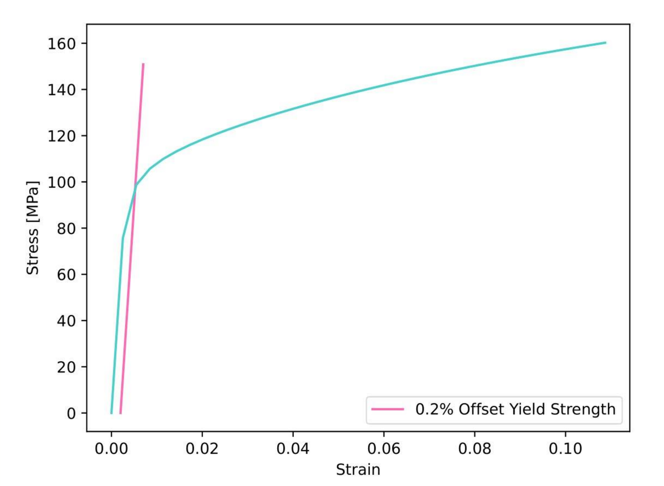


Figure 1. Plot of the average stress vs strain from a DAMASK simulation. The 0.2% offset is plotted and its intersection with the stress-strain curve indicates the yield stress value of the material.

- Crystal plasticity model DAMASK is used to evaluate the yield stress of a stochastically generated polycrystalline microstructure representative volume element (RVE) [3].
- The polycrystalline RVE is modelled as a Voronoi tessellation with 20 grains and the centroid and orientation of each grain is a uniformly distributed random variable.
- The attributions considered in a DAMASK simulation are listed below.

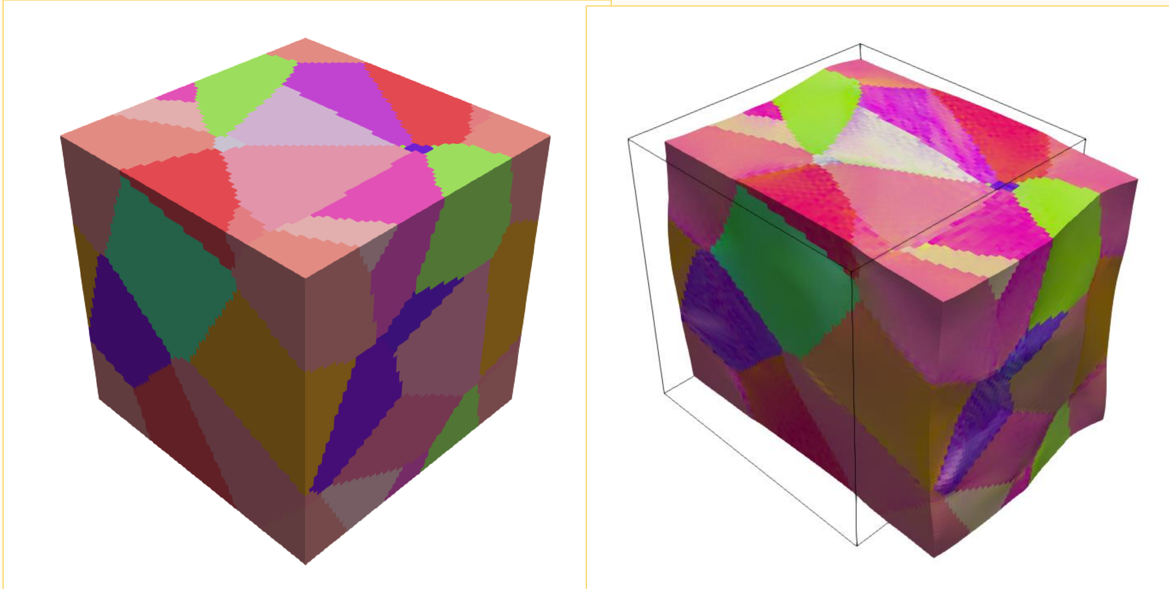
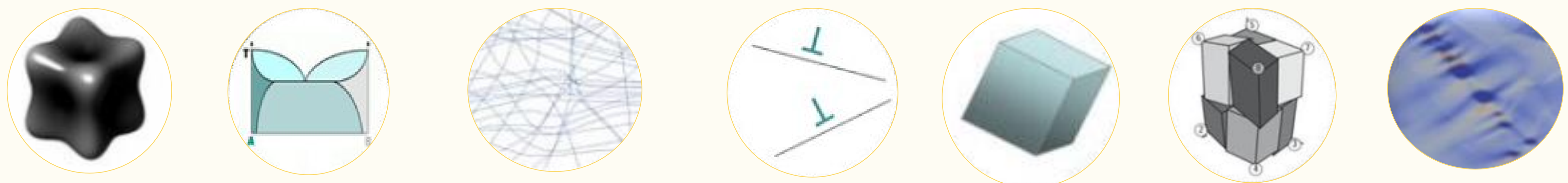


Figure 2. Left: Visualisation of a representative volume element (RVE) consisting of 20 grains. Right: The same RVE deformed by 10% strain along the X-direction.

- A uniaxial tensile load is applied and the RVE is deformed up to yield. The effective yield stress, evaluated using a 0.2% offset to the average stress-strain curve, is defined as the uncertain quantity of interest.



Elastic Tensor | Phase Fractions | Crystal Kinematics | Defect Dynamics | Orientation | Homogenization | Damage

Simulations of Failure Probabilities

- To evaluate the likelihood of plastic yielding under a given load in a material without physically testing lots of samples we simulate uniaxial deformation in a large number of RVEs using DAMASK and calculate the proportion that fail.

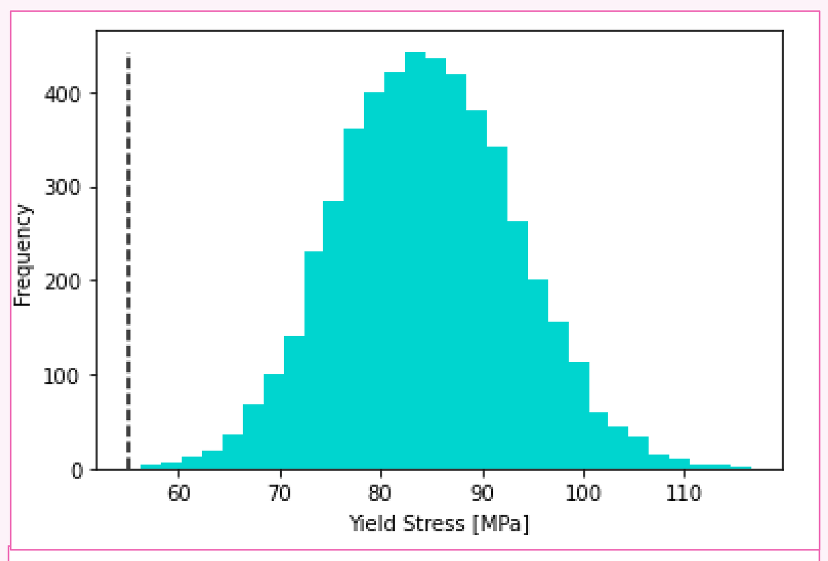


Figure 3. Monte Carlo simulation of magnesium yield stresses where N=10000 and the probability of failure = 0.0105 ± 0.0010

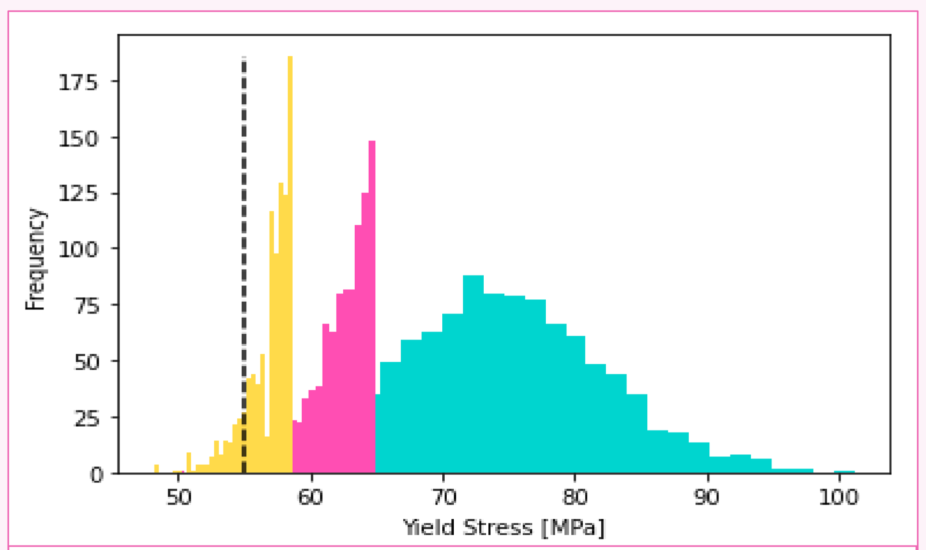


Figure 4. Subset simulation of magnesium yield stresses where N=1000, N levels = 3, spread = 0.05 and the probability of failure = 0.0015 ± 0.14

- Using direct Monte Carlo to sample the input RVE distribution resulted in a very computationally expensive approach. A batch size 10000 samples was required to calculate a probability of failure of 0.0105 ± 0.0010.
- Using a subset simulation method, which conditionally samples iterative failure domains, reduces the number of samples needed to evaluate a probability of failure to a similar level of accuracy [4].
- We ran subset simulation for different sizes of N to show the convergence of the probability of failure and the decreasing size of the coefficient of variation. Figure 5 shows a simulation using 3 levels of size 1000 [5].

$$Cov = \sqrt{\sum_i \delta_i^2} \qquad \delta_i = \sqrt{\left(\frac{1-p_i}{N \cdot p_i}\right) \cdot (1+\gamma)}$$

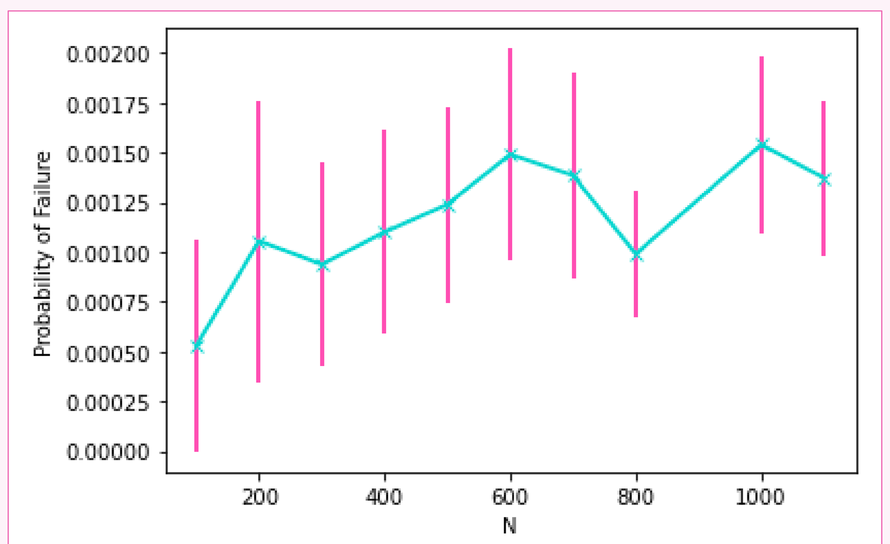


Figure 5. Probability of failure from subset simulation against the size (N) of each subset level

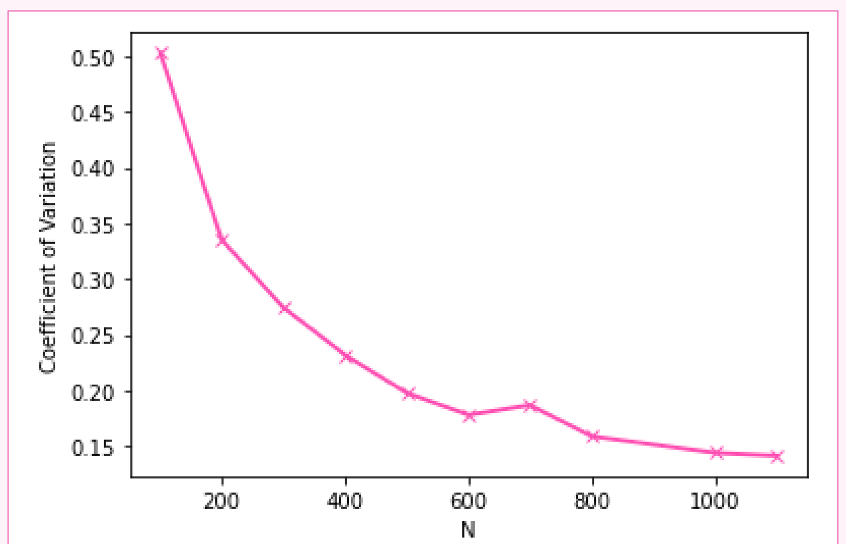


Figure 6. Coefficient of variation from subset simulation against the batch size (N) of each subset level

Conclusion and Next Steps

- We can model fusion materials using crystal plasticity and DAMASK to find yield stresses.
- Subset simulation gives an accurate probability of failure (plastic yielding) of a material using less computational power and time than direct Monte Carlo methods.
- The next step is to apply this to evaluate safe operating stress thresholds for a given acceptable probability of failure.

References and Acknowledgements

[1] Meade, D. (2010) 50 years of fusion research. *Nucl. Fusion.* 50, 1-14.
[2] Danson, C., and Gizzi, L. (2023) Inertial confinement fusion ignition achieved at the National Ignition Facility – an editorial. *High Power Laser Sci. Eng.*, 11, E40.
[3] Roters, F., et al. (2019) DAMASK – The Düsseldorf Advanced Material Simulation Kit for modelling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale. *Comput. Mater. Sci.*, 158, pp.420–478.
[4] Beck, J. and Au, S. (2001) Estimation of small failure probabilities in high dimensions by subset simulation, *Probabilistic Eng. Mec.*, 16, 4, 263-277.
[5] Behrensdorf, J. et al. (2023) UncertaintyQuantification.jl: A new Framework for Uncertainty Quantification in Julia, *5th ECCOMAS Thematic Conference on Uncertainty Quantification in Computational Sciences and Engineering.*

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