Uncertainty and multiphysics for predictive breeder blanket modelling

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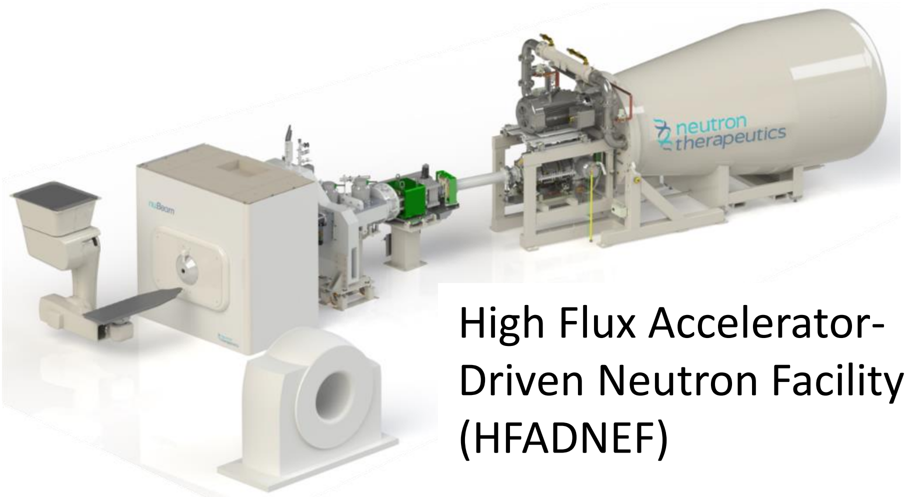
LiBRTI Conference on Breeder Blanket Technology
3rd-5th February 2026

TRIMAX – Tritium Reaction Integrated Multiphysics Analysis eXperiment

What is TRIMAX?

- Collaboration between University of Birmingham (UoB) & Bangor University on LiBRTI.
- UoB project aim: *Develop a small solid lithium ceramic breeder with in-line tritium detection capability for calibrated neutron sources*
- TRIMAX (Bangor) we are:
  - creating a general-purpose breeder blanket digital twin with Uncertainty Quantification (UQ)



High Flux Accelerator-Driven Neutron Facility (HFADNEF)

PRIFYSGOL BANGOR UNIVERSITY

NUCLEARFUTURES Bangor

TRIMAX – research breakdown

Digital twin Tom Griffiths	Review existing models	Design twin of experimental setup	Test, modify, validate
Uncertainty analysis Yehor Yudin	Review deficiencies in data and models	Incorporate uncertainty into digital twin	Identify key bottlenecks and critical parameters
Atomistic modelling Cillian Cockrell & Tom Smith	Review poorly understood physical processes	Perform simulations to provide data and physical insight	Implement new physics into the digital twin
Experimentation Elia Zancan	Review experimental methods	Perform experiments to characterise materials and measure tritium	Ameliorate digital twin with data and readings

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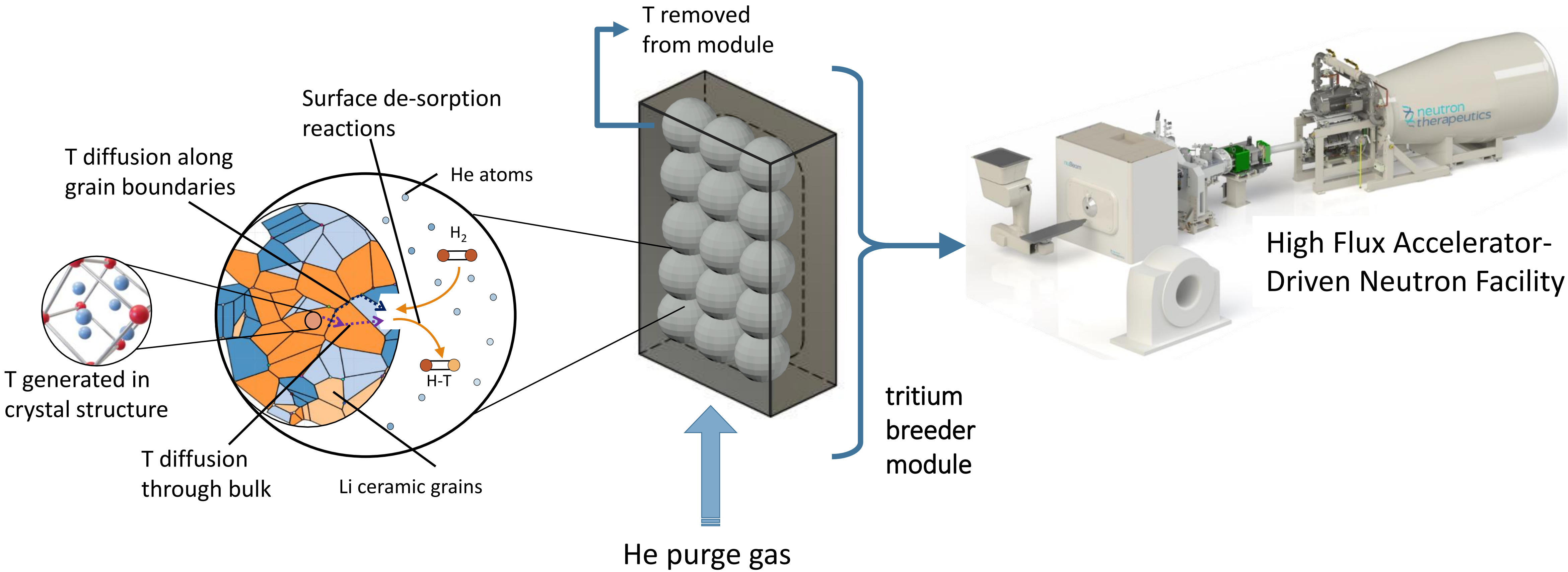
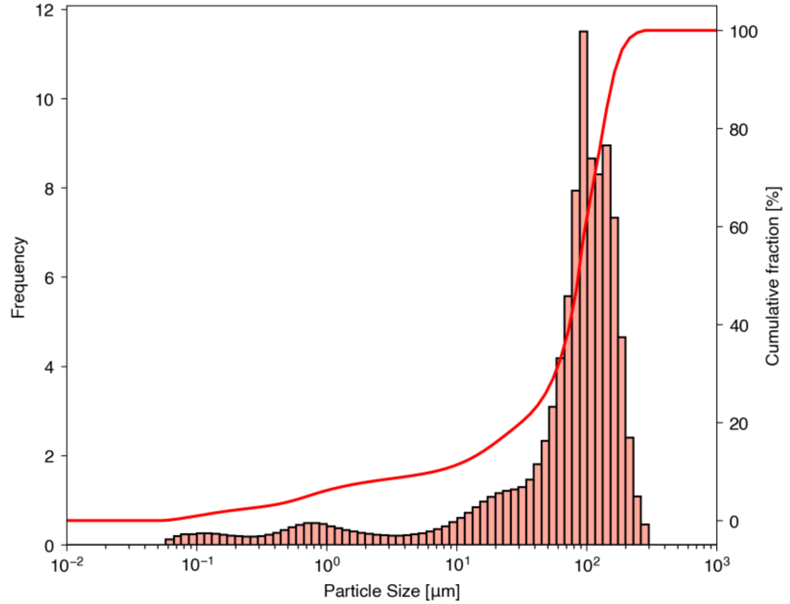
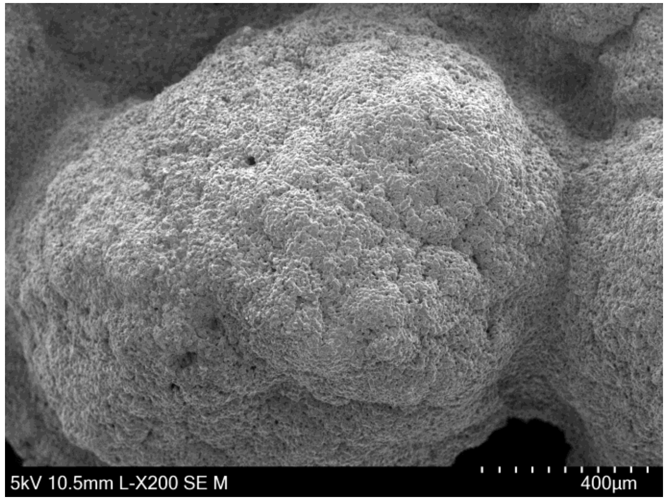
TRIMAX – Experimentation

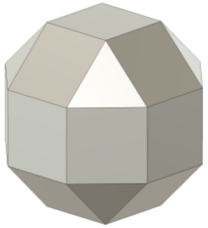


TRIMAX – Sample fabrication:

- Li_2TiO_3 kernels and monoblocks produced by sintering. Open porosity of 50%.
- Provided to UoB for irradiation and characterisation.

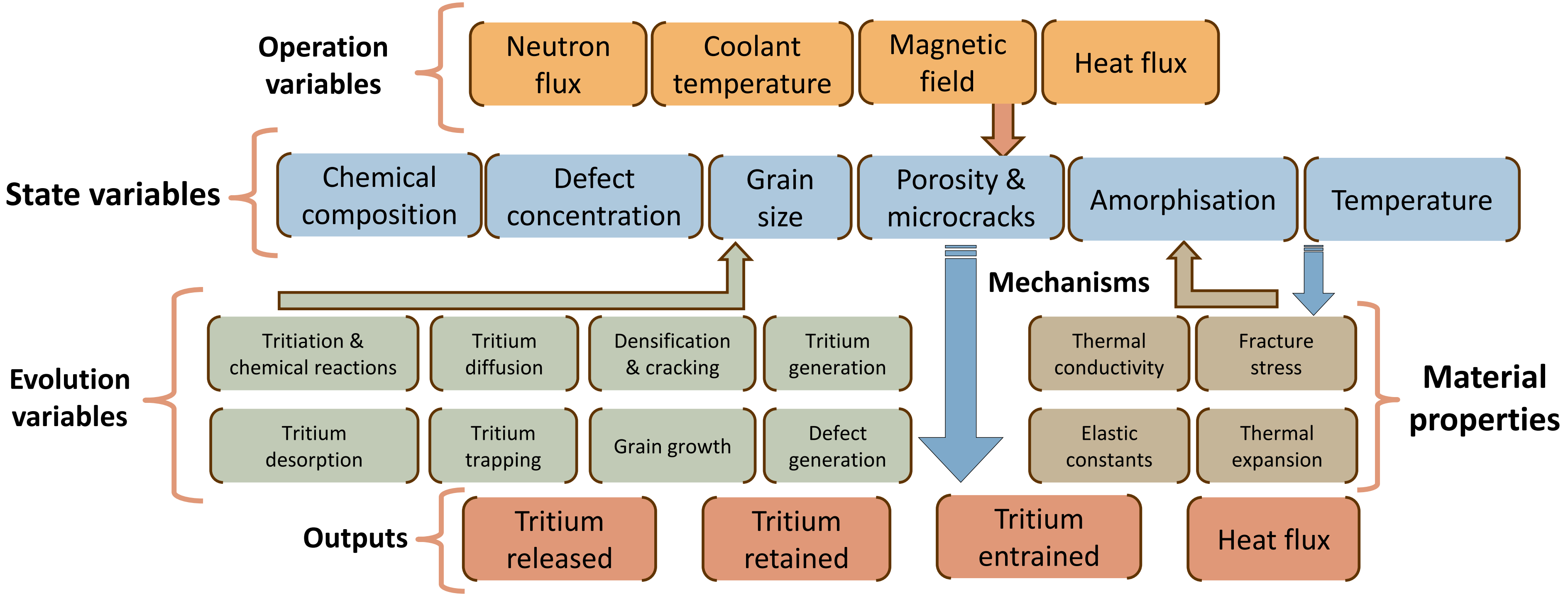






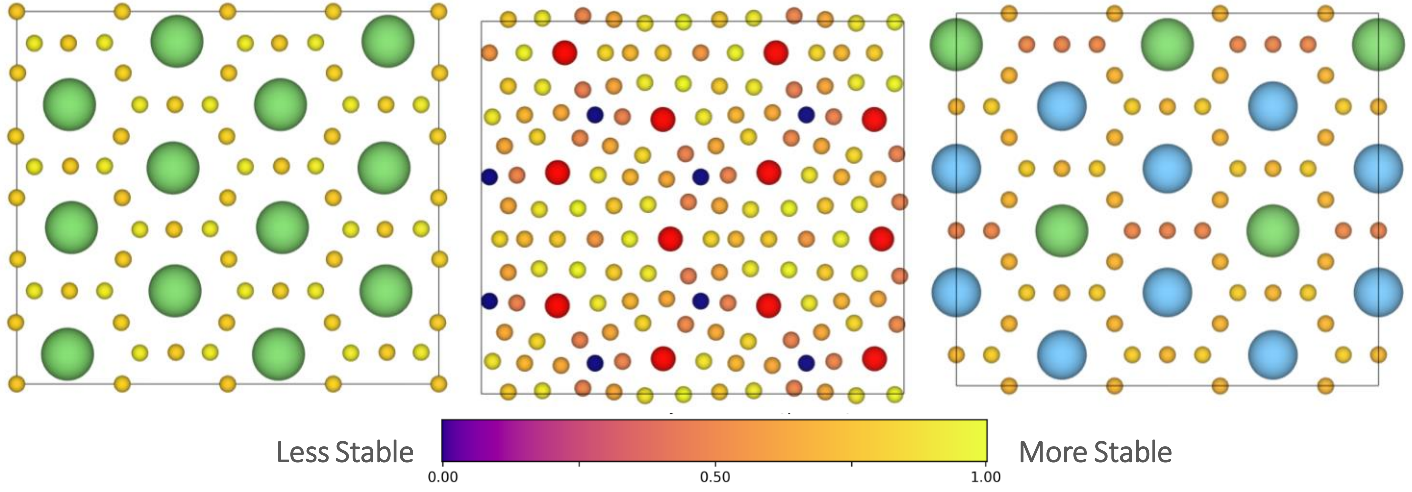
Dr. Elia Zancan

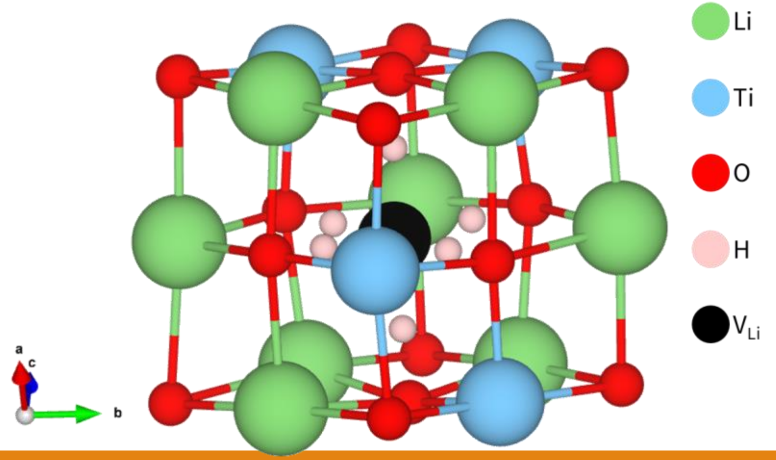
TRIMAX – parameters & predictions



TRIMAX – DFT:

- Geometry optimisation for defect formation energies.
- Climbing-image nudged elastic band calculations for diffusion/trap energy barriers.
- Vibrational calculations for kinetic coefficients.
- Evaluate different pathways for each transition.

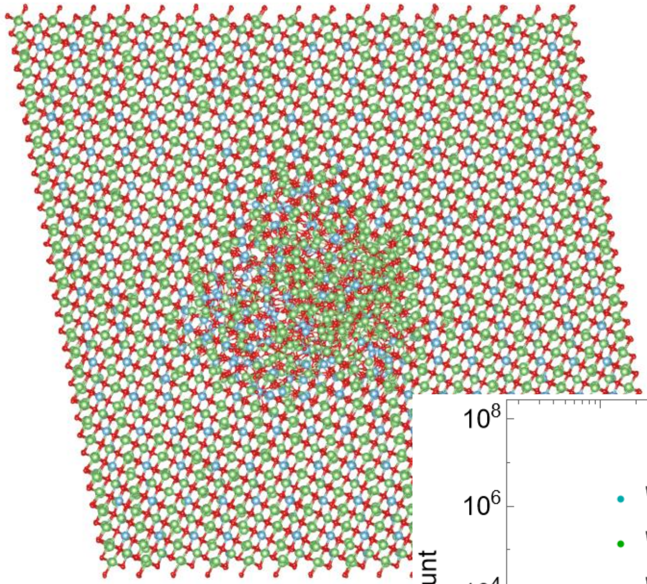


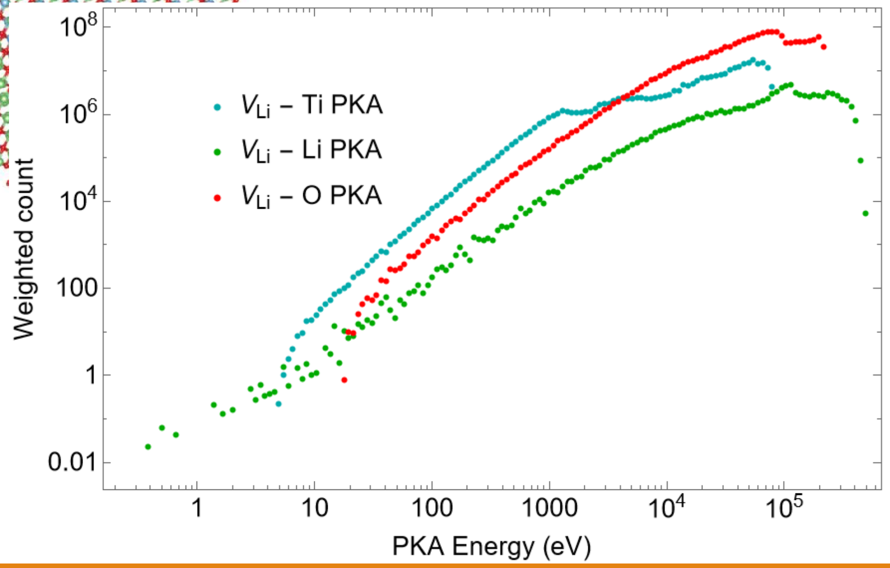


Dr Tom Smith

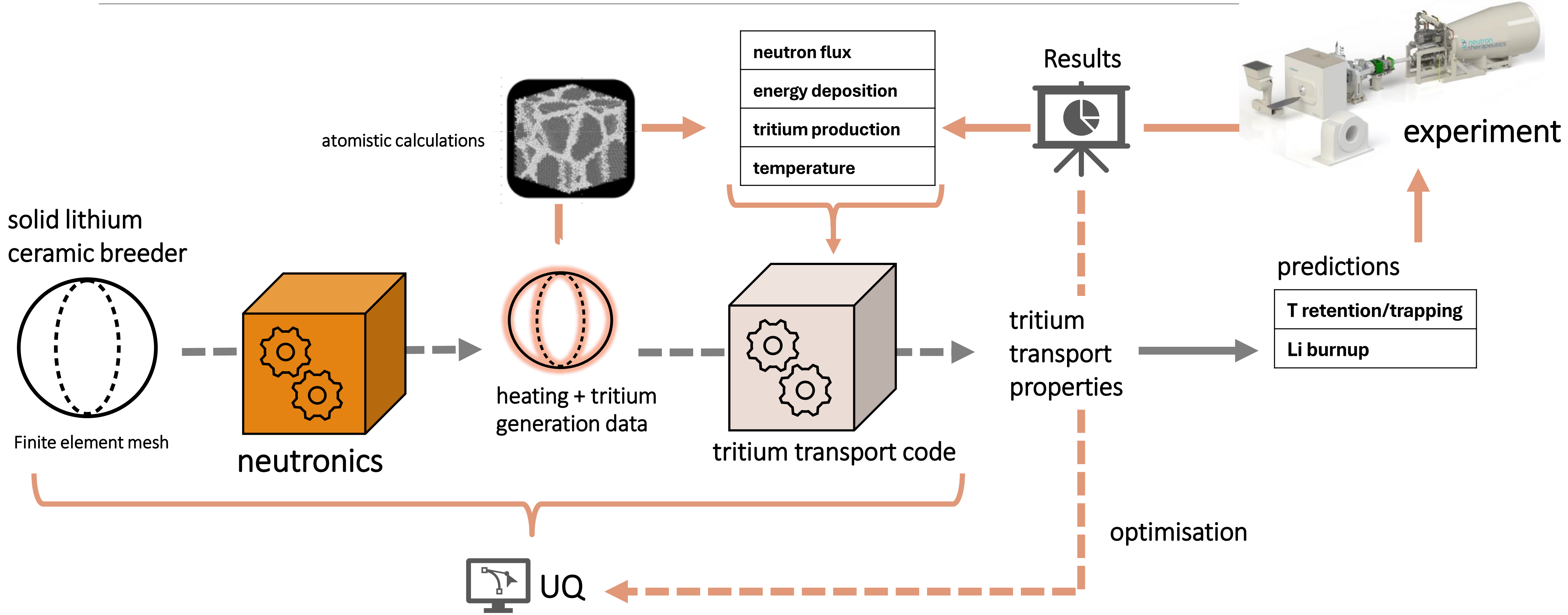
TRIMAX – Molecular dynamics:

- Defect production as a function of incident energy from radiation cascade simulations.
- PKA distribution for different species from neutronics.
- Combined for defect traps as a function of fluence in the sample.
- Machine-learnt interatomic potentials to accelerate diffusion calculations and increase fidelity of cascade simulations.





TRIMAX – Digital twin overview



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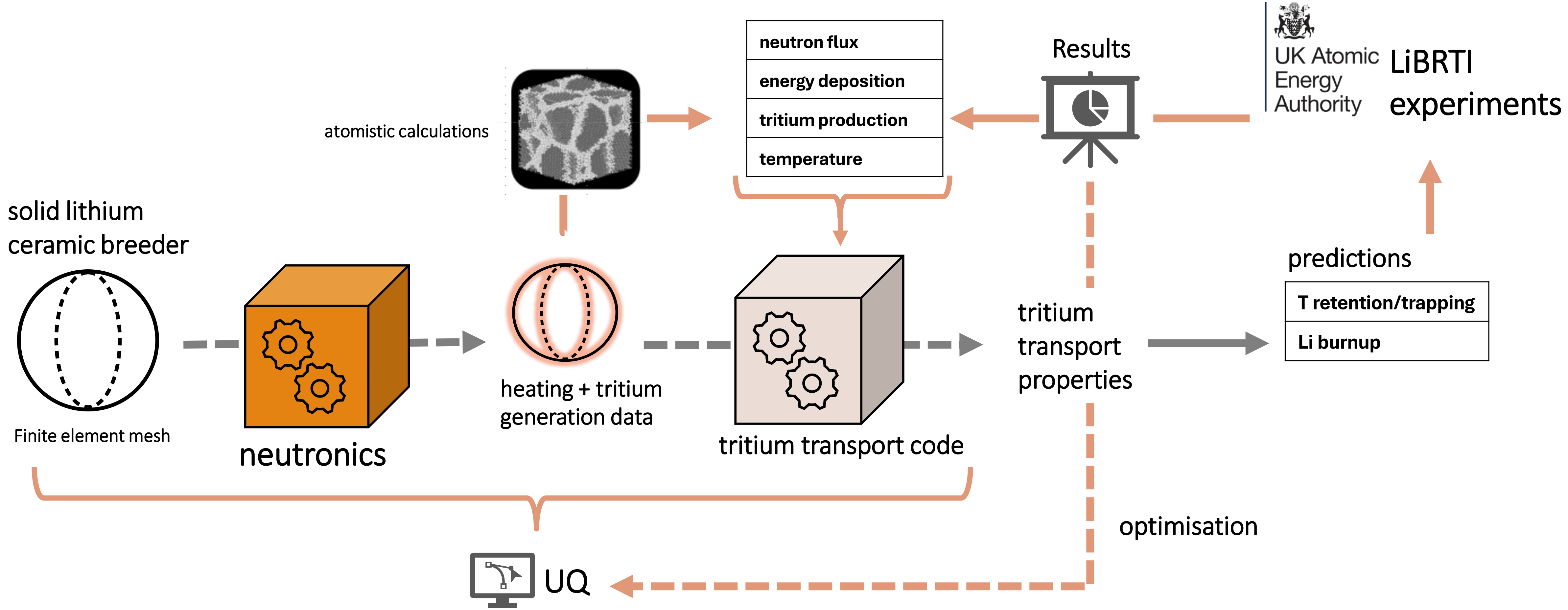
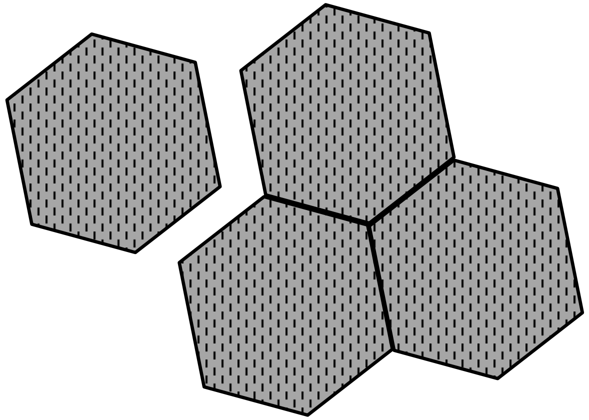


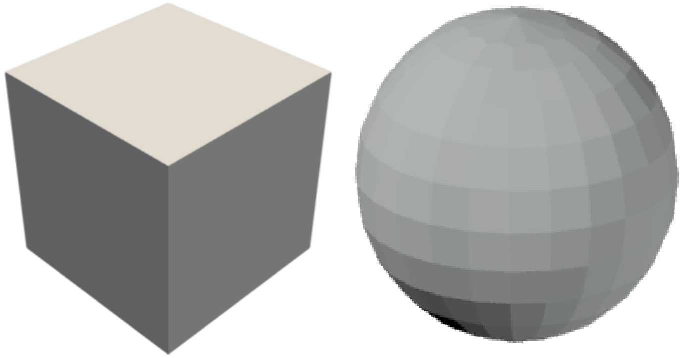
TRIMAX – different scales

microscale:



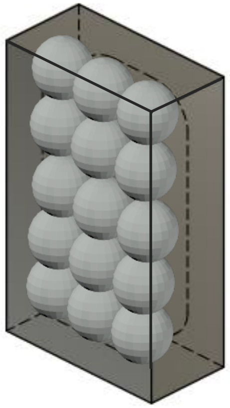
small group crystal grains

mesoscale:



large group of crystal grains

macroscale:

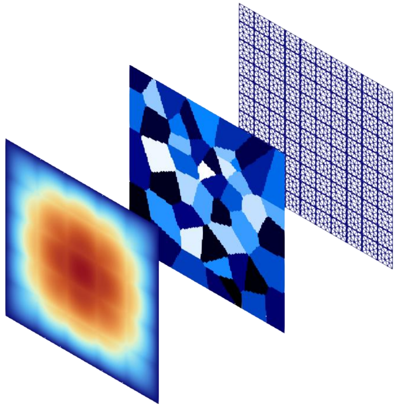


a breeder module

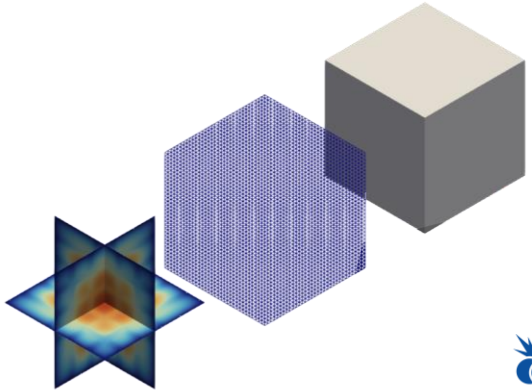
TRIMAX – different scales

MOOSE framework enables scaling from 2D to 3D

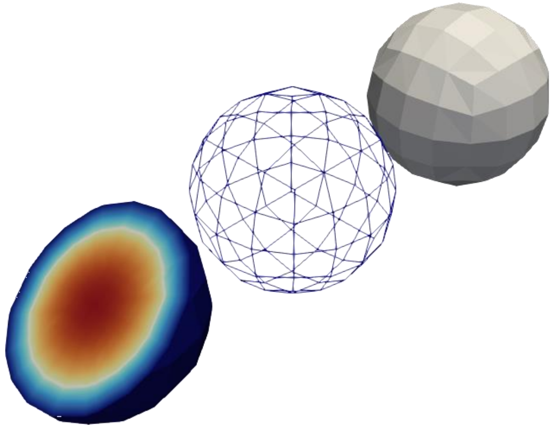
microscale:



mesoscale:



macroscale:



FESTIM
FINITE ELEMENT SIMULATION OF TRITIUM IN MATERIALS

MOOSE

TMAP8

SALAMANDER

TRIMAX – microscale simulations

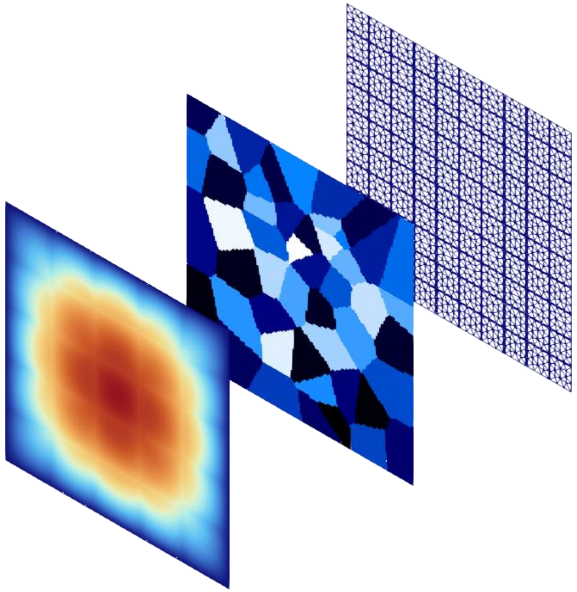
2D

40 microns

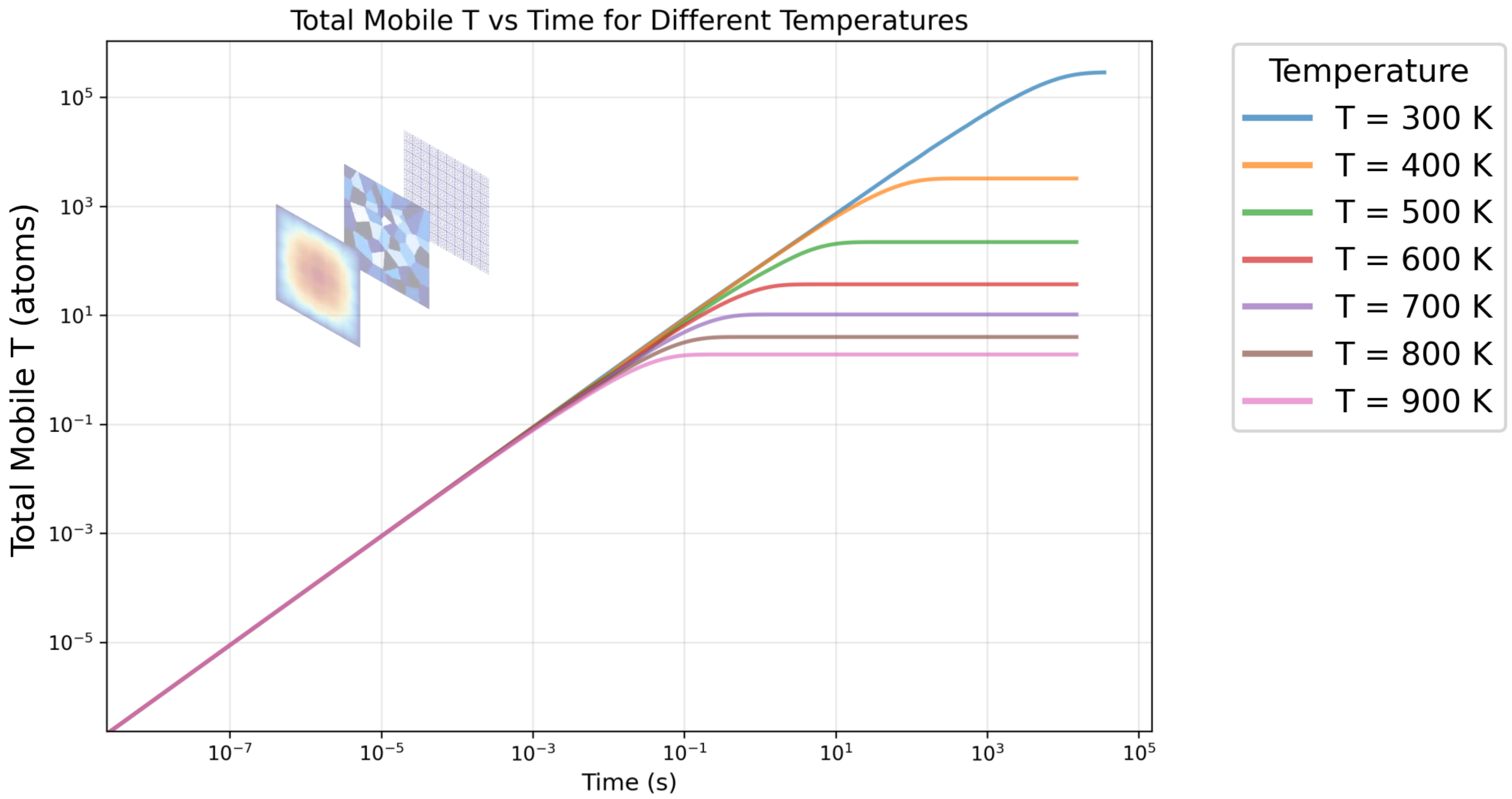
Time to reach stead-state for:

- mobile tritium
- trapped tritium
- tritium flux

As a function of temperature



TRIMAX – microscale simulations



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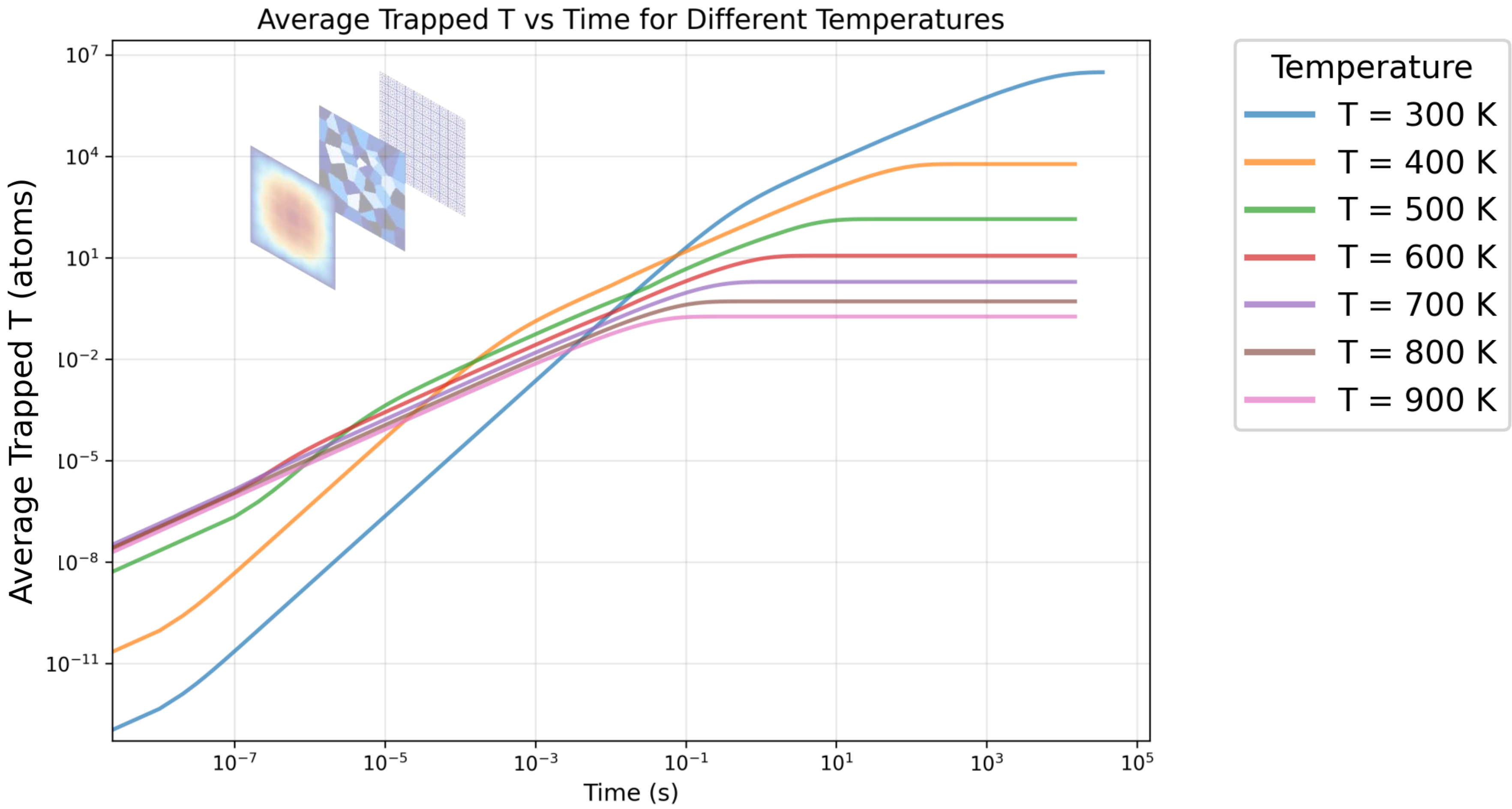

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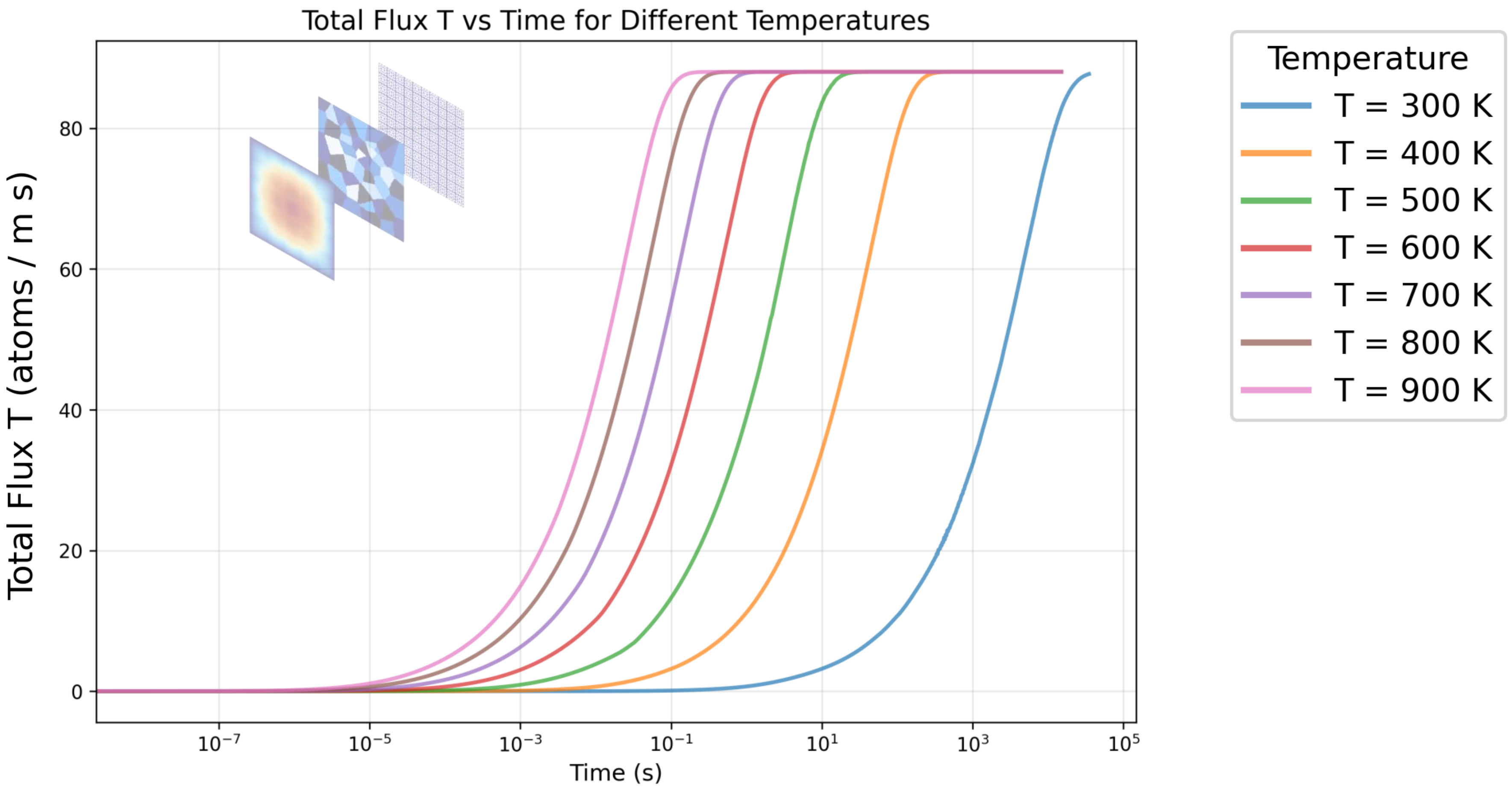


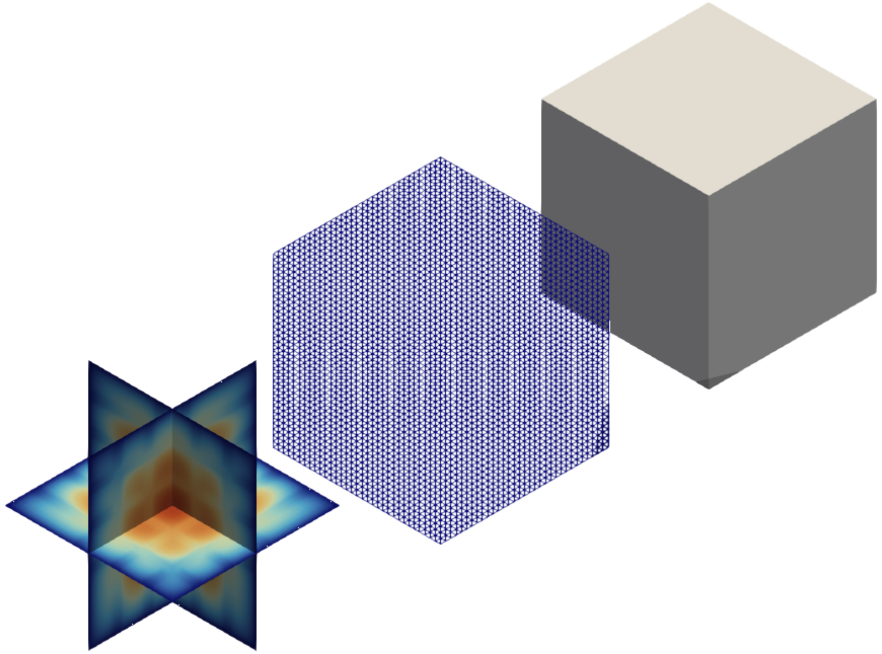
TRIMAX – microscale simulations

3D

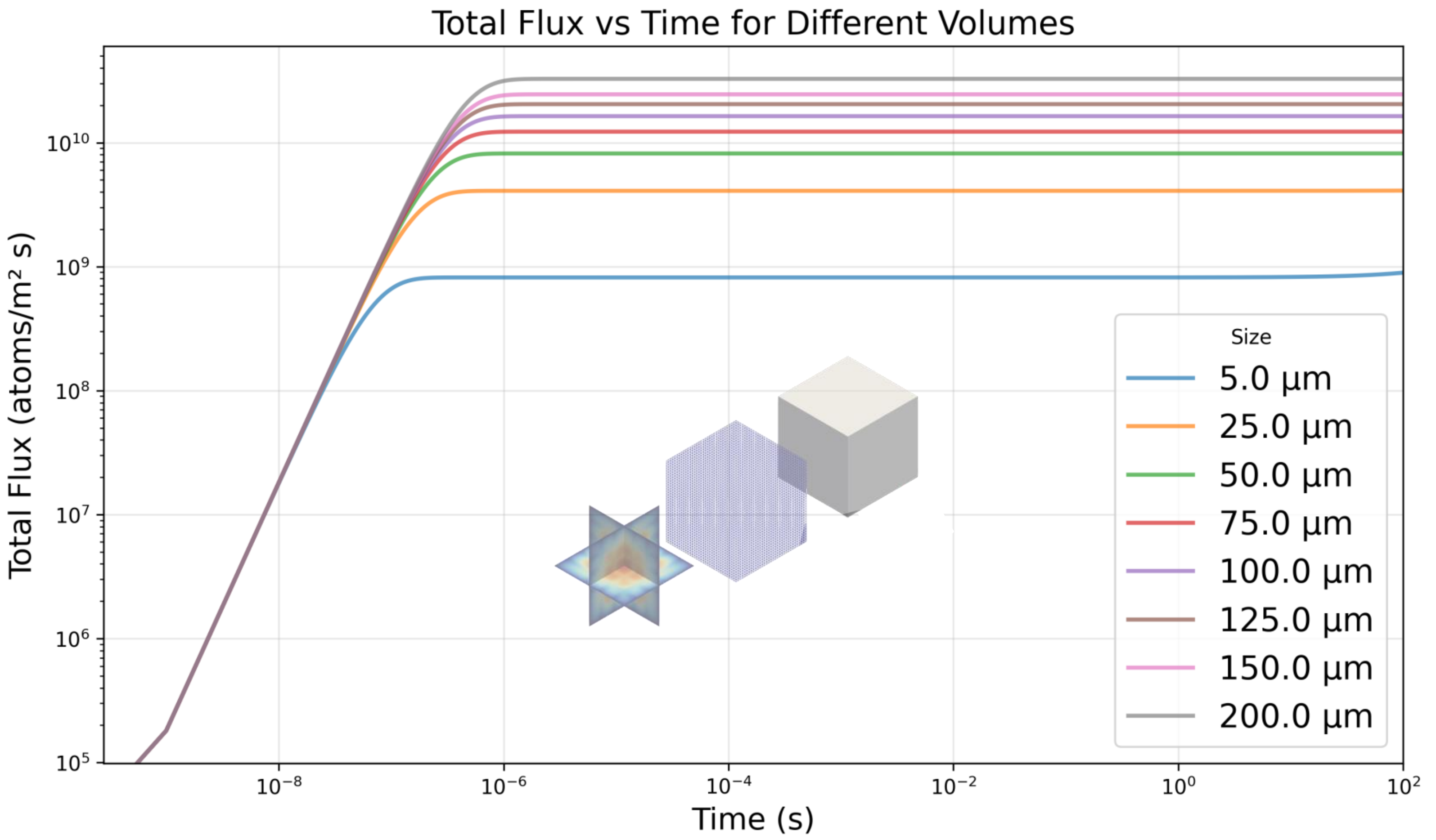
Time to reach steady state for:

- Tritium flux

As a function of total **volume**



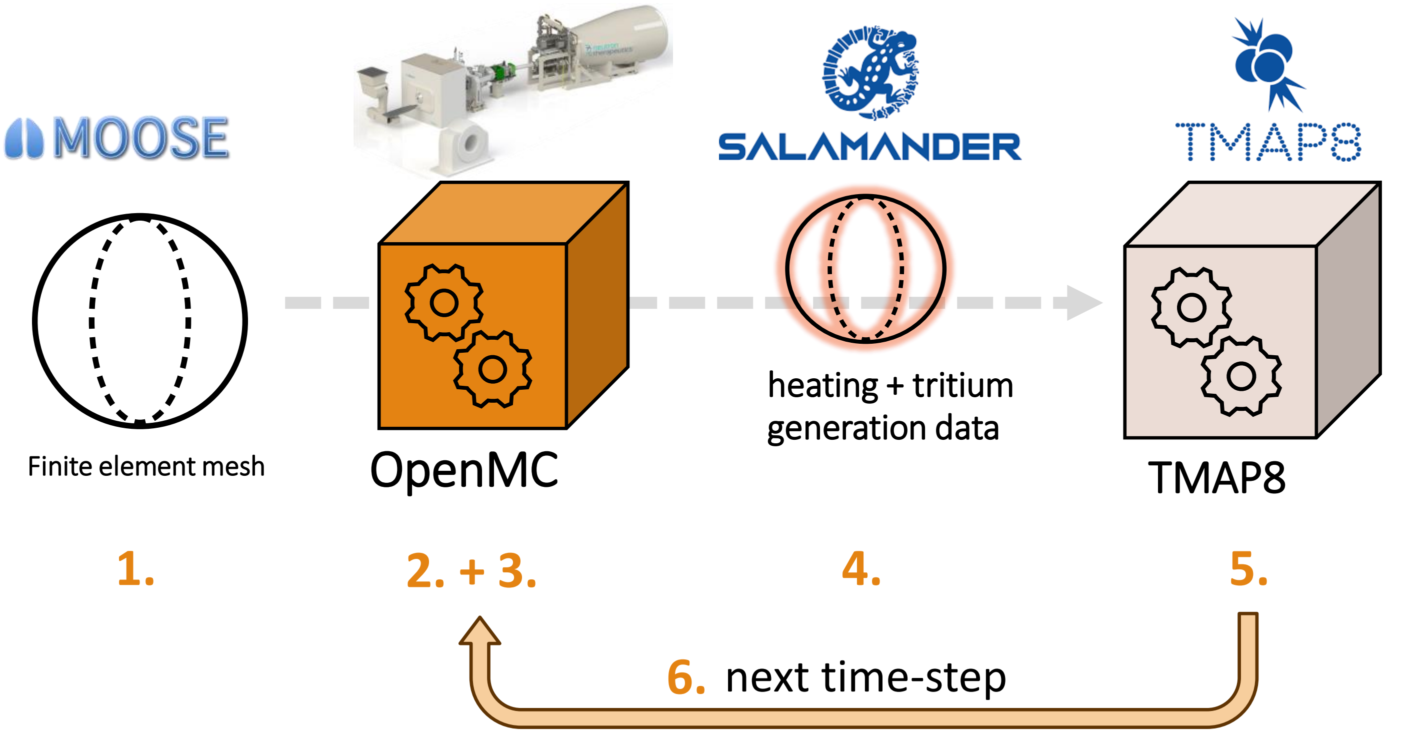
TRIMAX – microscale simulations



TRIMAX – macroscale online coupling:

next time-step

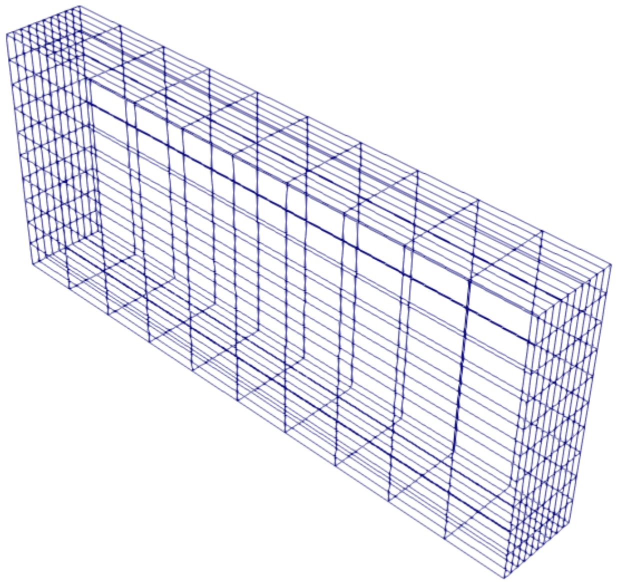
1. MOOSE loads mesh
2. Cardinal initializes OpenMC
3. OpenMC reads HF-ADNeF source at first time-step
4. SALAMANDER transfers heating/tritium → initialises TMAP8
5. TMAP8 solves diffusion at first time-step
6. TMAP8 transfers heat transfer data back to OpenMC



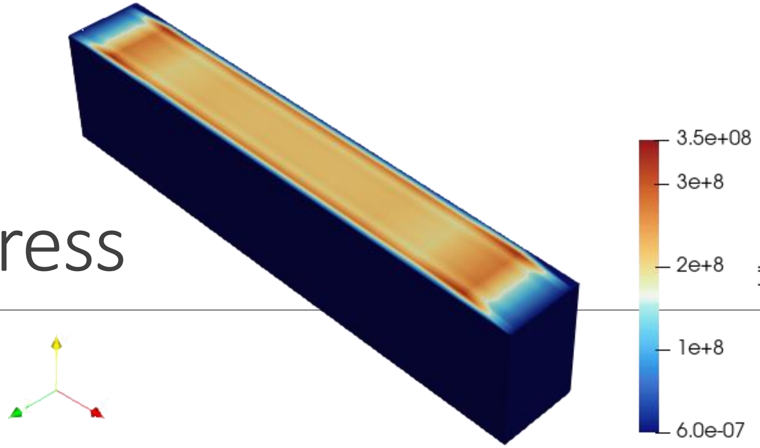
TRIMAX – macroscale simulations

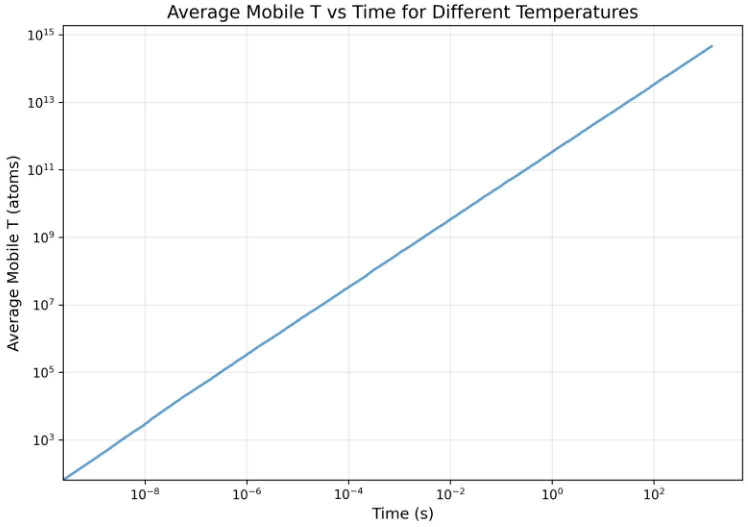
Geometry:

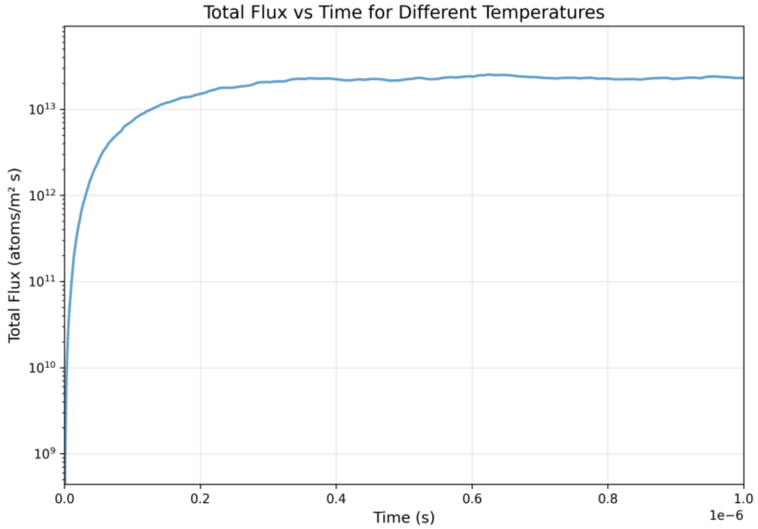
- Dimensions: 3D
- Monoblock volume = 20 cm^3
- Homogeneous titanate material
- 900s (time in UoB beam-line)

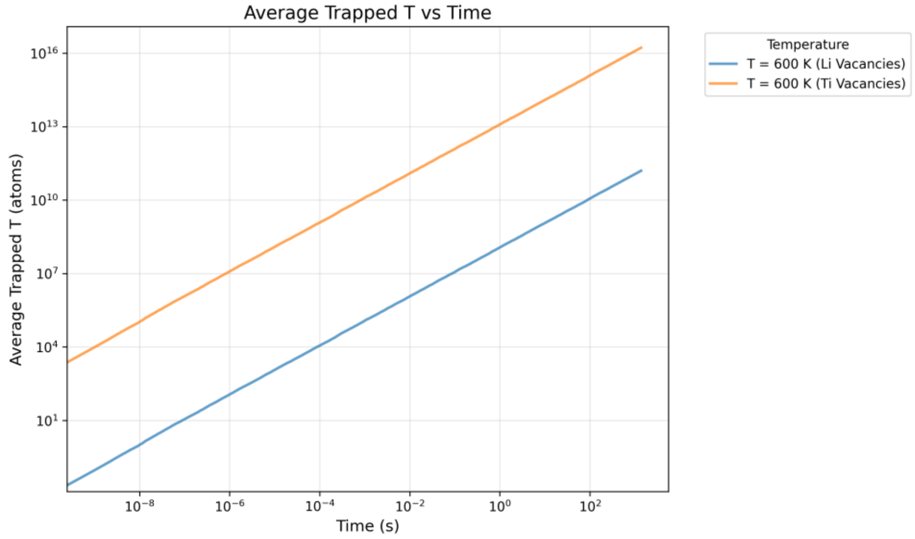


TRIMAX – Work in-progress









TRIMAX – Intermediate outlook:

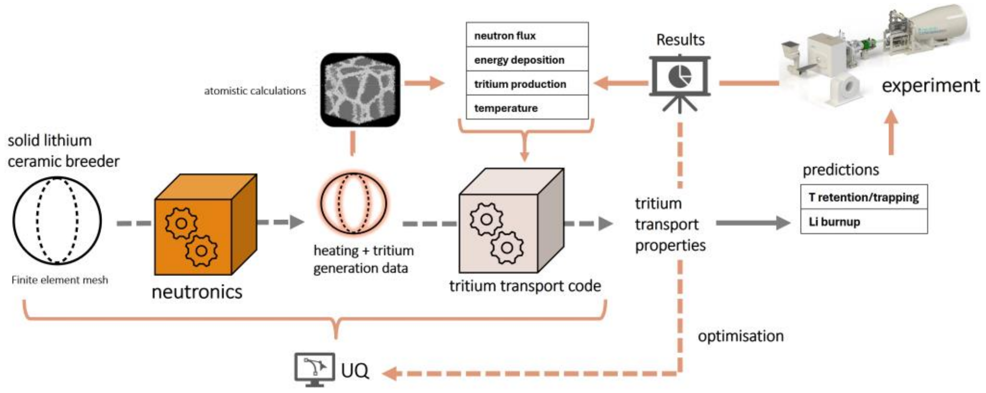
- Our macroscale simulations use a homogeneous block of titanate material – simplistic
  - We will capture more of the microscale physics
- Compile coupled model on HPC for UQ and sensitivity analysis

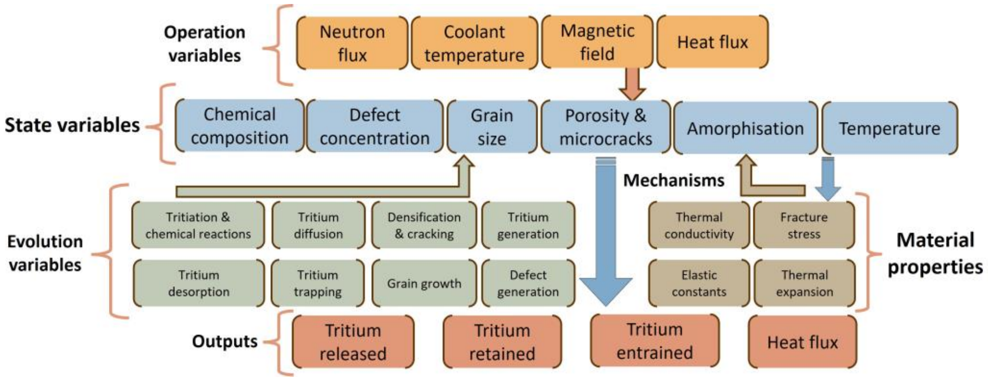
Long term:

- Include CFD for the helium purge gas
- Consideration of higher flux sources and larger breeder modules

TRIMAX – Intermediate summary:

- We have developed an all-purpose digital twin for lithium ceramics that combines:
  - Molecular dynamics
  - Evolving microstructure
  - Tritium transport
  - Neutronics
- An operating code for LiBRTI





TRIMAX – Tritium Reaction Integrated Multiphysics Analysis eXperiment

- How do we treat the uncertainty of an inaccessible and exploratory setup?

- Experimental / operational uncertainty:
  - How much tritium will be released and trapped?
  - How sure are we about material and engineering conditions?
  - Are there any unaccounted factors influencing behaviour of components?

- Model / theoretical uncertainty:
  - How does parameter knowledge affect predictions?
  - How does model structure influence prediction uncertainties?
  - How do modelled conditions affect observables?

Uncertainty Quantification

I. Lack of knowledge and/or understanding

II. Assign *probability* measure for outcomes

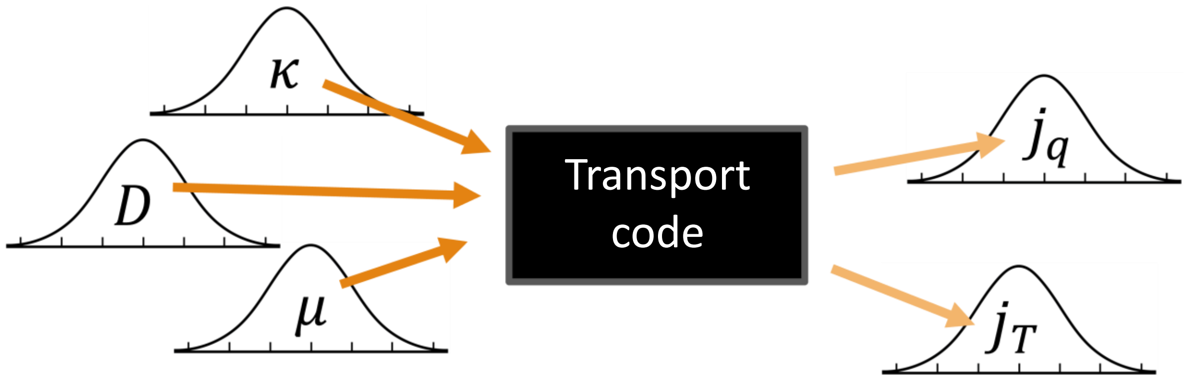
- Use probability theory to formulate problem
- and relevant numerical algorithms to quantify results

Variety of methods of *Uncertainty Quantification (UQ)*

- Non-intrusive: based on multiple deterministic runs (Monte Carlo, Polynomial Chaos Expansion, Gaussian Process Regression)
- Intrusive: construct model considering terms can be stochastic (Stochastic FEM)

Variety of issues:

- Computational cost!
- Incorporate uncertainties of different types
- Interpret results



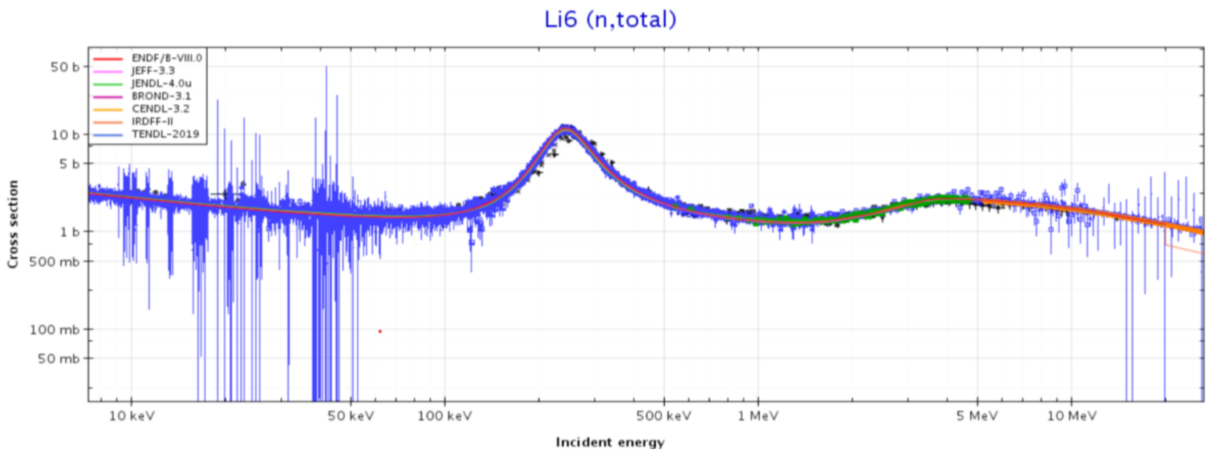
Uncertainty sources

Sources vs Phenomenon or quantity	Fundamental Empirical Data	Experimental difficulty	Modelling aspects
Neutronics: cross-sections	$\sigma: Li-6(n,t)$ IMPORTANT	Experimental dependant – could vary order of magnitude	Needs to be propagated through model, per case → $\boldsymbol{G(x,t)},\ \boldsymbol{Q_V(x,t)}$
Material Evolution	Experiments difficult to extrapolate	Post-experimental assessment	Need simulation and propagation through scales per case: *information propagation*
Material Properties	Some 'table' values are accurate	From very small to basically never measured	Computed at atomistic scale and propagated → $\boldsymbol{D_0\ (x,t), E_d(x,t)}$; ***BC parameters***
Engineering parameters	Experiment dependent	Constraints and a level of control, mostly before experiment	Has to be studied consistently: $\boldsymbol{R_{max}, T_{amb}}$, *etc.*
TBR	All factors included	Macroscopic QoI that incorporates all quantities (out of scope of the experiment)	Literature: DEMO[1]: $\Delta_{FC} \approx 0.05, \Delta_{CM} \approx 0.1$ LOTUS[2]: $1.4-35.8$ [%]

[1] DEMO: U. Fischer, FED 98–99 (2015) 2134–2137 *[2]* LOTUS: J. Stepenek, doi: 10.13182/FST86-A24856

Neutronics: data and model uncertainty

- OpenmMC computation
- Uncertainty Sources:
  - MC noise → can be *reduced*
  - Nuclear DB data uncertainty
- Average quantities from *preliminary* simulations[*]:



JANIS view of DBs for (n,X) reactions cross-section for 6Li

Ceramics:

- $G_T = 1.16 \cdot 10^8 \pm \mathbf{7.84}\% \left[\frac{T}{mA}\right]$
- $Q = 9.09 \cdot 10^5 \pm \mathbf{11.57}\% \left[\frac{W}{mA}\right]$

Air:

- $G_T = 0 \left[\frac{T}{mA}\right]$
- $Q = 3.68 \cdot 10^{-7} \pm \mathbf{61.8}\% \left[\frac{W}{mA}\right]$

<u>Input</u>: energy spectrum, material and layout, cross-section data. *<u>Output</u>*:

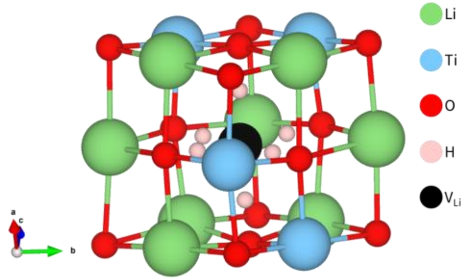
Explanation	Symbol	Unit (OpenMC)	Mean value	Relative STD [%]
Tritium tally/production	$G_T(E_n)$	$(mA)^{-1}$	$2.90 \cdot 10^7$	$\mathbf{80.4}$
Neutron flux	$\Gamma_n(E_n)$	$(mA)^{-1}$	$4.19 \cdot 10^9$	$\mathbf{53.3}$
Heat generation	$Q(E_n)$	$W\ (mA)^{-1}$	$2.51 \cdot 10^5$	$\mathbf{91.0}$

[*] L. Butt at UoB

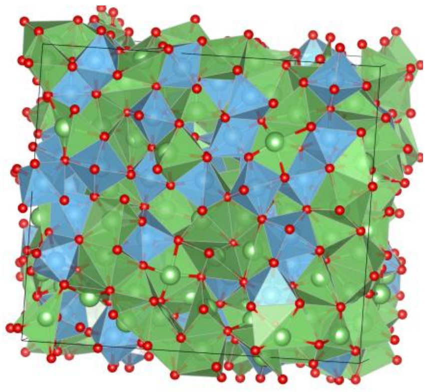
Uncertainty sources in atomistic simulations

Density Functional Theory (DFT):

- Potential form:
  - Aleatoric:
    - Bifurcations between pathways etc.
  - Epistemic:
    - Empiric potential fitting: Bayesian regression variance; etc
  - Approximations:
    - LDA, GGA, …
- Statistics:
    - Finite size of the system
    - Fraction of defects, pathways etc. on a larger scale



Hydrogen cluster vacancy
[by T. Smith, T. Davey]



Lithium metatitanate, amorphous
[by C. Cockrell]

Molecular dynamics (MD):

- Statistical errors:
  - Event Count Number N_{ev}, $E \sim N_{ev}^{-\frac{1}{2}}$
    - Size of problem
    - Time of run
    - Irreducible: transition characteristics
  - Likelihood extrapolation
- Approximations, parameter uncertainty…
- Translation to pore and grain level:
  - Grain parameters distribution

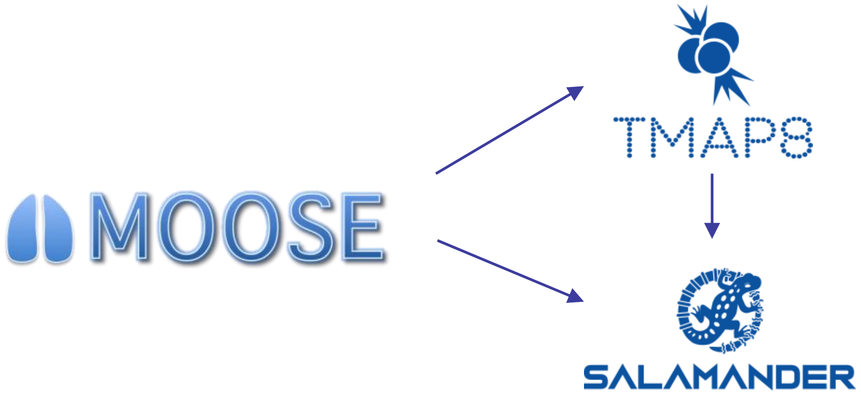
Gas transport models

I) Based on *FESTIM 2.0 [1]*

- Functionality:
  - 1D/3D in plane/cylindrical/spherical coord-s
  - Coupled with heat diffusion
  - Boundary: surface kinetics, convective + radiative cooling

II) Based on TMAP8 (*MOOSE) [2,3]*

- *SALAMANDER [4]* : coupling with neutronics via Cardinal: *OpenMC [5]*
- Functionality:
  - 2D/3D
  - Domains with different phases (bulk/boundary)
  - Multi-species
  - Realistic sources (*SALAMANDER* coupling)
  - Boundary: recombination flux
  - Trapping: single species



[1] https://github.com/festim-dev/FESTIM
[2] https://github.com/idaholab/TMAP8
[3] https://github.com/idaholab/moose
[4] https://github.com/idaholab/salamander
[5] https://github.com/openmc-dev/openmc

Uncertainty Quantification: gas build-up in a grain

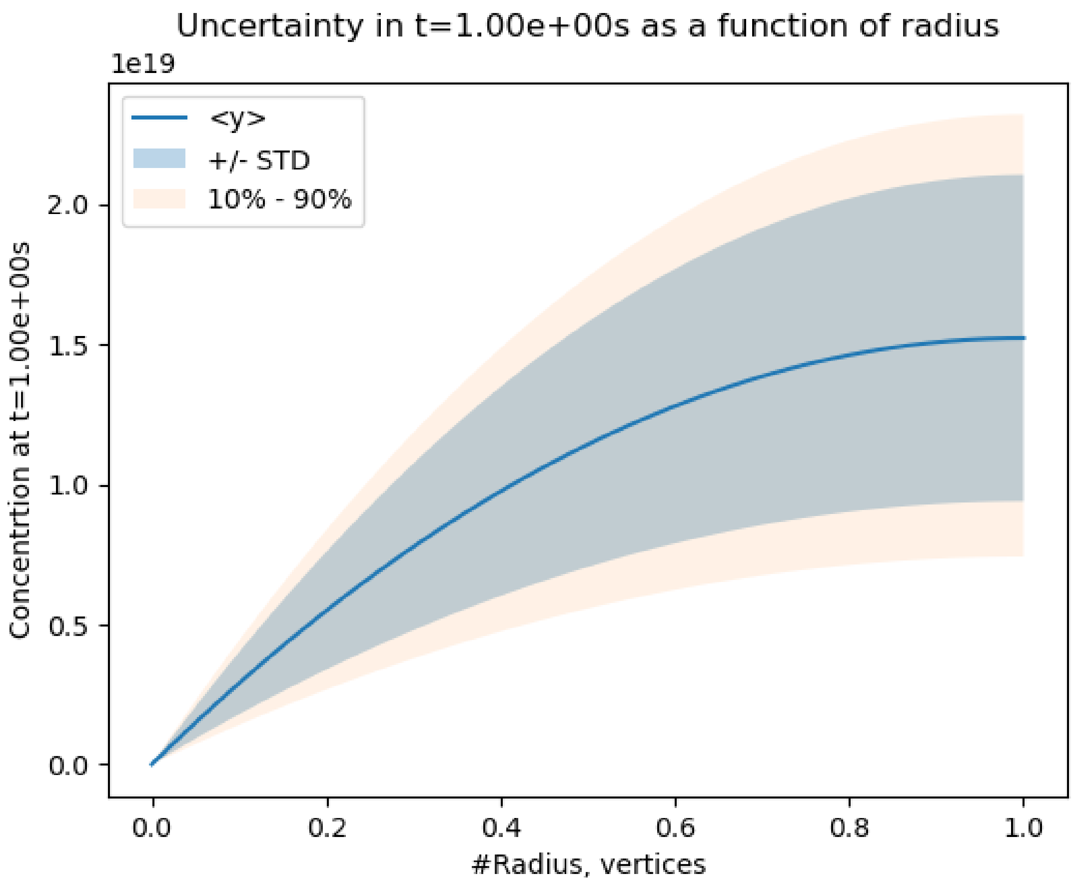
Example: continuum FEM material modelling
(FESTIM-NIUQ *[1]*: 2nd order PCE method via EasyVVUQ *[2]* applied to FESTIM2 model)

Sources of uncertainty: *Relative Input Uncertainty* $= 0.25$

- Material properties: diffusion coefficient D_0
  → Atomistic simulations
  → material choice and design
- Ambient conditions: Temperature T_{amb}
  → Engineering calculations/data
  → possibility of two-side feedback
- Combination:
  Boundary Condition: Concentration at Boundary $C_T^{BC}(R)$

Computed quantities:

- Tritium retention: tritium build-up $C_T(r)$
- Here: potentially up to $\mathbf{30\%}$ ***uncertainty***

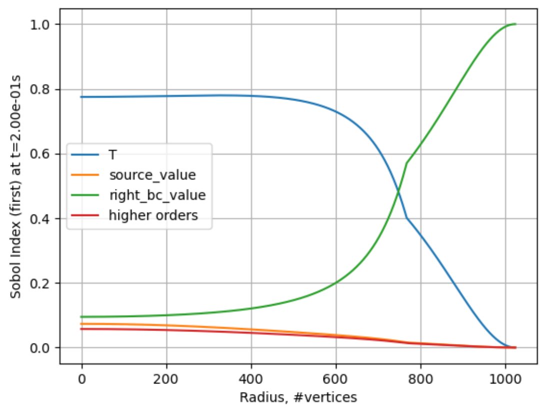


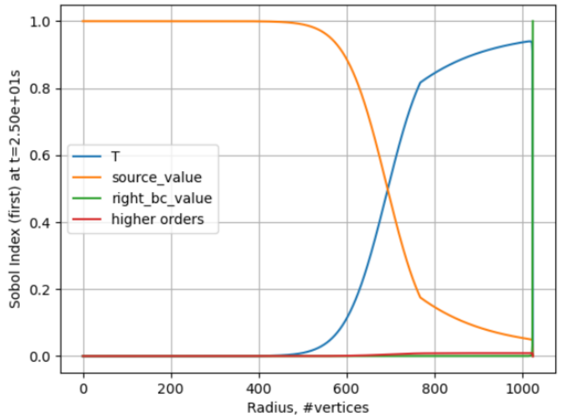
[1] https://github.com/YehorYudinIPP/festim_niuq
[2] https://github.com/UCL-CCS/EasyVVUQ

Sensitivity Analysis

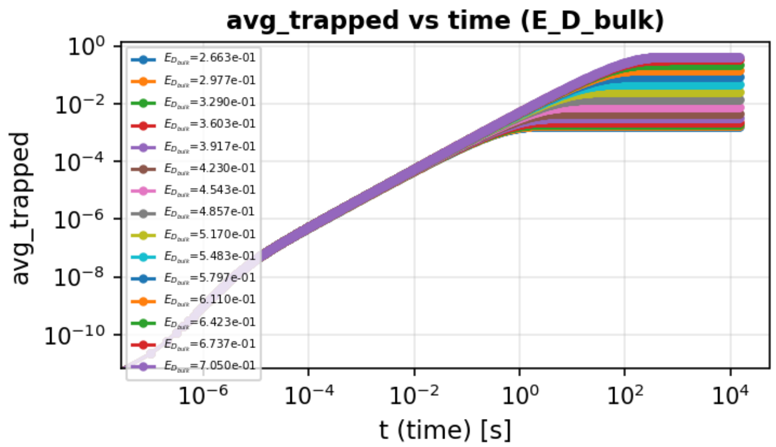
- …Which parameters' uncertainties have highest contribution to the outcome uncertainties?
- …Which parameters' change have highest contribution to the outcome change?
- …Which parameters are most important?

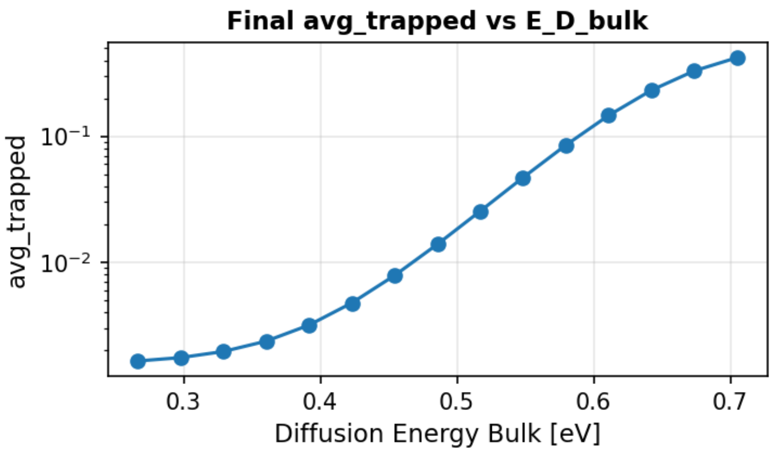
- Via *ANOVA (Analysis of Variance)* in terms of *Sobol indices*
- Most of (quadrature-based) UQ methods automatically support SA
- Help in Design of Experiment, Optimisation, etc.
- Here:
  - influence of different material properties and different conditions
  - coefficients of PCE used for UQ provide Sobol indices too
  - different size of samples show different sensitivity profiles

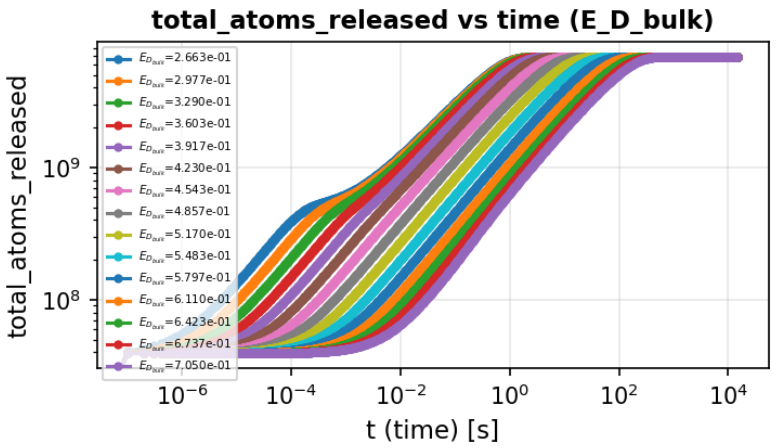




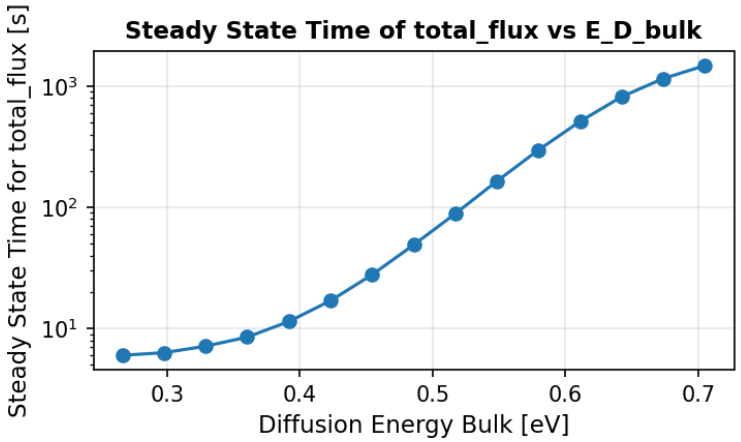
TMAP8 model scaling: activation energies – trapping, release, timescales







Crystaline bulk



Timescale:

dependent on E_D^{bulk}, $E_D^{g.b.}$

steady state in $t \approx 5 - 1000\ [s]$

approx.

$E_D^{bulk}: +0.1[eV] \rightarrow t_{s.s.}[s]: \times\ 10$

$E_D^{g.b.}:\ +0.3[eV] \rightarrow t_{s.s.}[s]: \times\ 10$

Trapping:

$\log \mathrm{N_{tr}} \sim E_D^{bulk}$

$\log \mathrm{N_{tr}} \sim E_D^{gr.b.}$

$E_D^{bulk}:\ +0.1[eV] \rightarrow N_{tr}[at.]: \times\ 10$

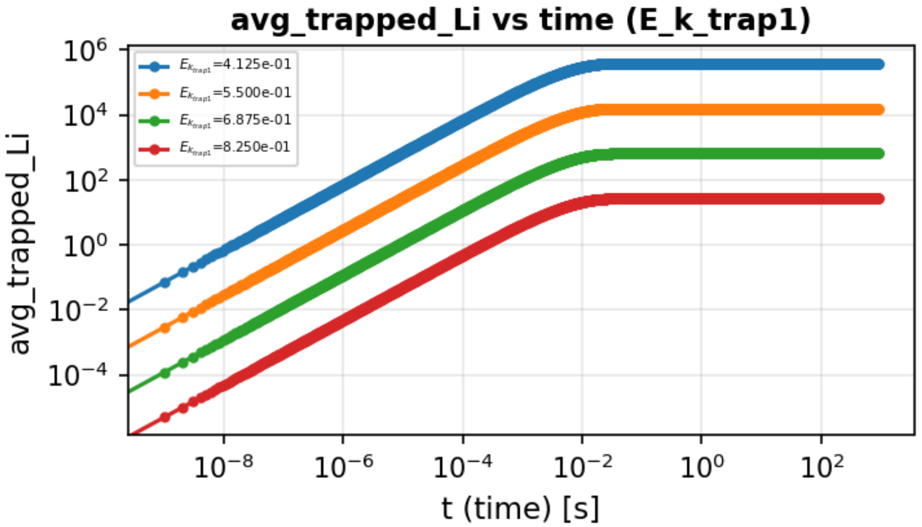
$E_D^{g.b.}:\ +0.3[eV] \rightarrow N_{tr}[at.]: \times\ 10$

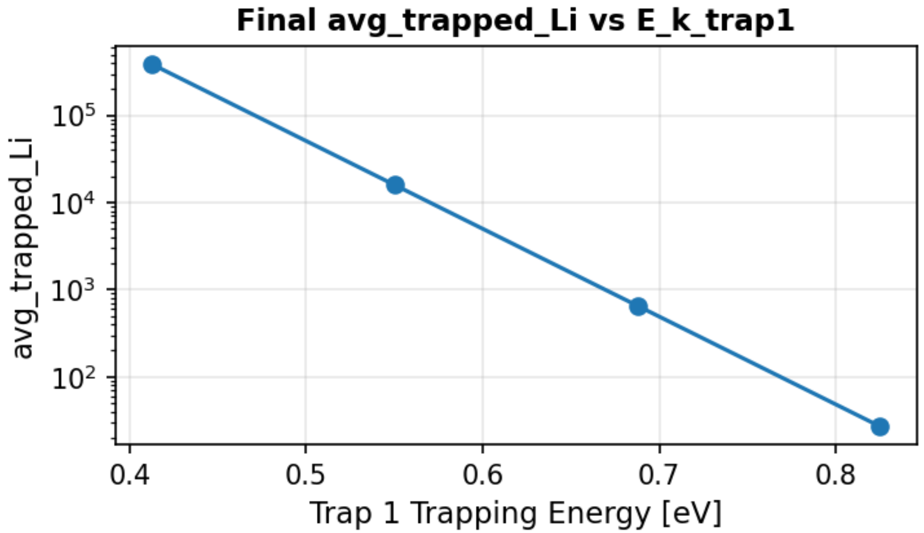
Release:

$\mathrm{m_{T-r}} \sim \boldsymbol{const}$

functional forms?

TMAP8 model scaling: Li & Ti trapping / de-trapping energies, trapping sites





Timescale:
steady state in $t \approx 1[s]$
(almost no dependency)

Trapping / De-trapping:
$\ln \mathrm{N_{tr}} \approx -23\ E_{tr}$
$\ln \mathrm{N_{tr}} \approx 23\ E_{dtr}$
$(\pm 0.1[eV] \rightarrow \times\ 10)$

$\mathrm{N_{tr}} \approx \boldsymbol{t.s.f.}$

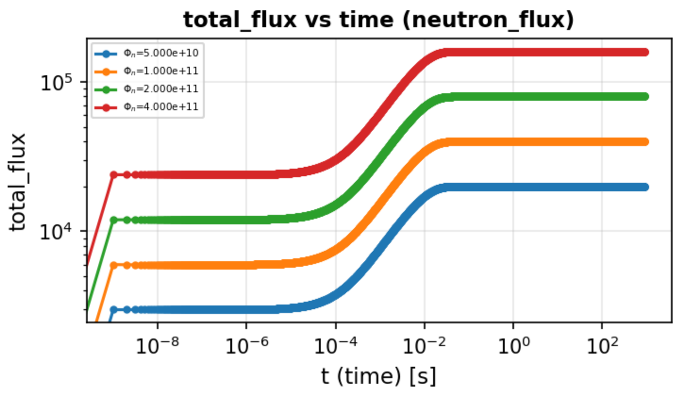
Sensitivities + interactions?

Li traps

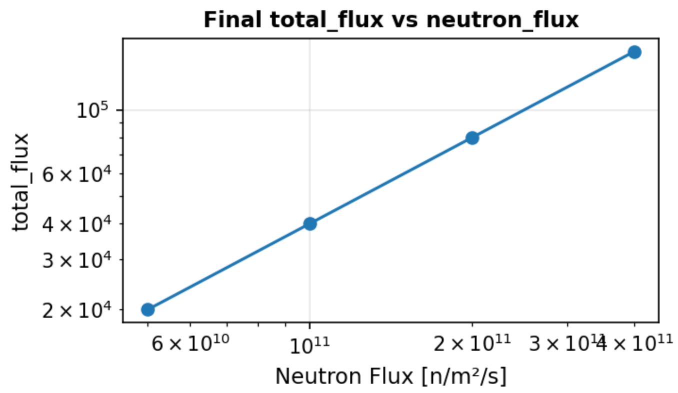
TMAP8 model scaling: neutron flux source - release

Tritium released vs t

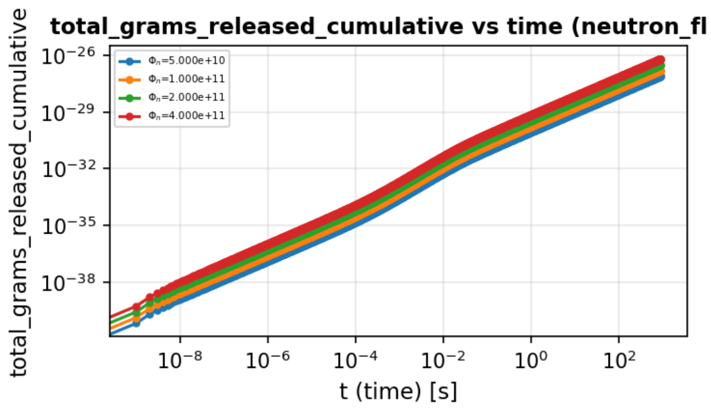
Neutron flux → Tritium atoms per $m^2 s$

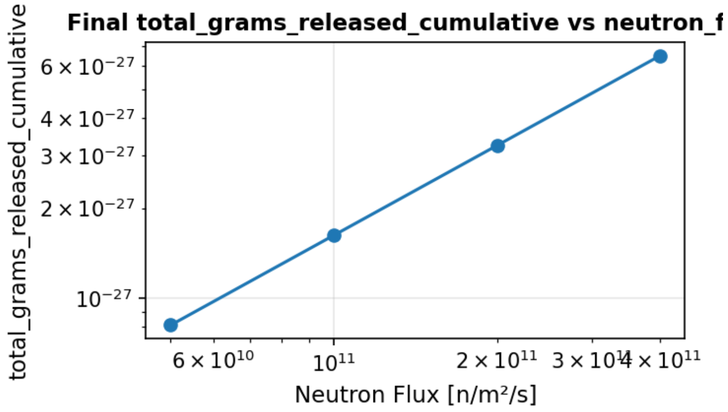


Tritium released vs value



Neutron flux → Tritium atoms total





Timescale:

steady state in $t \approx 1[s]$
(almost no dependency)

Released Tritium:

$\mathrm{N_{T-r}}, \mathrm{m_{T-r}} \sim \Phi_n$

Cumulative Released Tritium:

$m^{tot}_{\mathrm{T-r}} = \int_{t_0}^{t} m_{T-r}(t)\, dt \sim \Phi_n \cdot t$
(dynamics fast enough for initial stage not to matter)

Higher fidelity?
Interactions?
Correlations?

TMAP8 model scaling: energies, trapping, neutronics

Parameter	Range	*Effect*
Trapping & de-trapping energy, E_{dtr} , E_{tr}	E_{tr}^{Li} $[eV]$: $0.4 - 0.8$; E_{tr}^{Ti} $[eV]$: $0.8 - 1.6$ $E_{dtr}^{Li}[eV]$: $0.6 - 1.1$; $E_{dtr}^{Ti}[eV]$: $1.6 - 3.0$	$E_{dtr/tr} \pm 0.1[eV] \rightarrow \times\, 10\ \mathrm{N_{tr}}$ [at.]
Activation energy in bulk & boundary, E_D^{bulk}, $E_D^{g.b.}$	$E_D^{bulk}[eV]$: $0.25 - 0.7$ $E_D^{g.b.}$ $[eV]$: $0.25 - 0.6$	E_D^{bulk} $+ 0.1[eV] \rightarrow \times\, 10\ \mathrm{N_{tr}}$ [at.] , $\times\ \mathbf{10}\ \boldsymbol{t_{s.s.}}$ $[\boldsymbol{s}]$ $E_D^{g.b.}$ $+ 0.3[eV] \rightarrow \times\, 10\ \mathrm{N_{tr}}$ [at.], $\times\ \mathbf{10}\ \boldsymbol{t_{s.s.}}$ $[\boldsymbol{s}]$
Trapping site fraction, $t.s.f.$	$t.s.f._{\mathrm{Li}}$ $[\mathrm{fr.}]$: $10^{-6} - 10^{-5}$ $t.s.f._{\mathrm{Ti}}$ $[\mathrm{fr.}]$: $10^{-7} - 10^{-6}$	$\mathrm{N_{tr}} \sim t.s.f.$
Neutron Flux, Φ_n	$\Phi_n[n\, m^{-2} s^{-1}]$: $10^9 - 10^{14}$	$\mathbf{N_{tr}}, \mathbf{N_{rel}} \sim \boldsymbol{\Phi_n}$

MOOSE STM: Uncertainty Quantification

Stochastic Tools Module (STM) *[1]:*

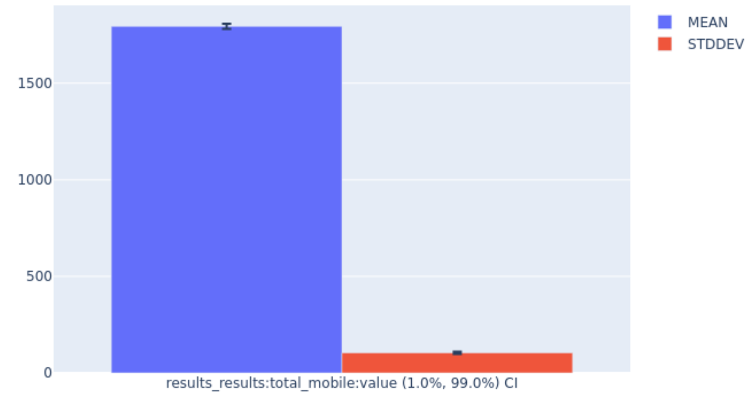
- Monte Carlo (MC), Polynomial Chaos Expansion (PCE)
- Parametric studies
- Sensitivity: Sobol indices
- Surrogate types: PCE (regression, quadrature), Gaussian Process (GPR)
- Surrogate methods: create, train, evaluate, validate, compare
- Dimensionality reduction: Principal Orthogonal Decomposition (POD)
- Potential: Bayesian Model Selection

Uncertainty source:

$T, \Gamma_n \pm 10\%, E_D^{bulk}, E_D^{g.b.} \pm 20\%$

Method:

MC (Saltelli) sampling

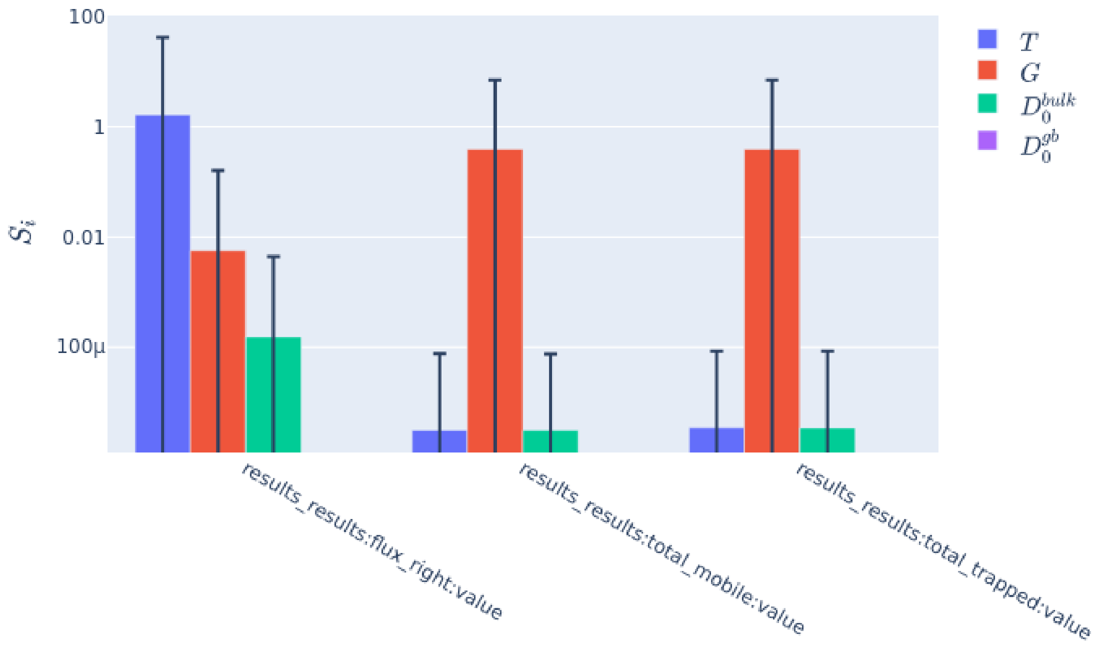


Mean and standard deviation ($\pm$ MC error) for total mobile inventory

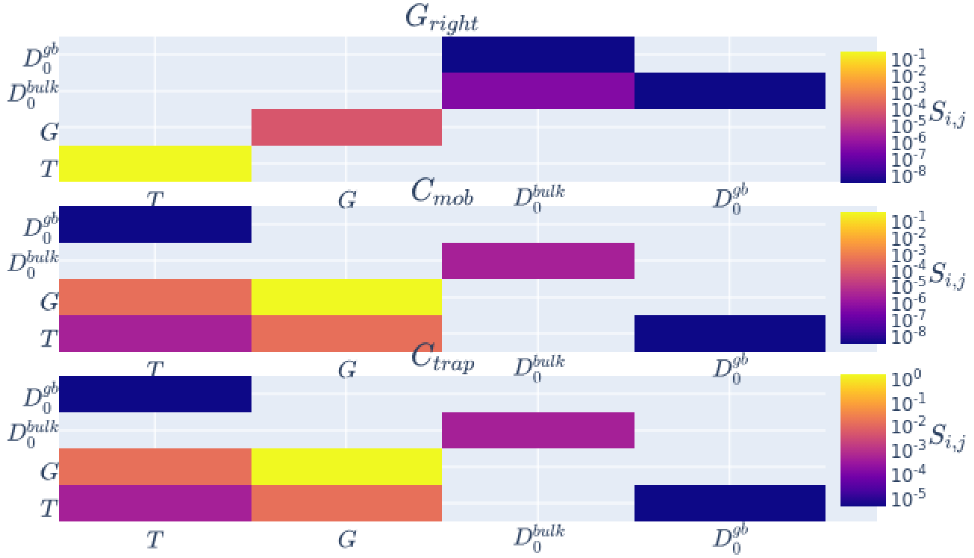
Quantity	Mean	Mean(1-99%)	STD	STD(1-99%)
$C_{mob}^{tot}\ [m^{-3}]$	$1.79 \cdot 10^3$	$(1.79 - 1.81) \cdot 10^3$	**104.0**	$(197.6 - 109)$
$\Gamma_T\ [s^{-1}m^{-3}]$	$1.7 \cdot 10^{-3}$	$(1.46 - 1.95) \cdot 10^{-3}$	$\mathbf{1.92 \cdot 10^{-3}}$	$(1.72 - 2.09) \cdot 10^{-3}$

[1] https://mooseframework.inl.gov/modules/stochastic_tools

MOOSE STM: Sensitivity Analysis



Sobol indices for flux, mobile, trapped T as a function of temperature, source, diffusivity at bulk and boundaries



Second order Sobol indices for combinations of parameters

Inverse UQ: Bayesian model selection

Bayesian inference/calibration

Update believe given experimental data:

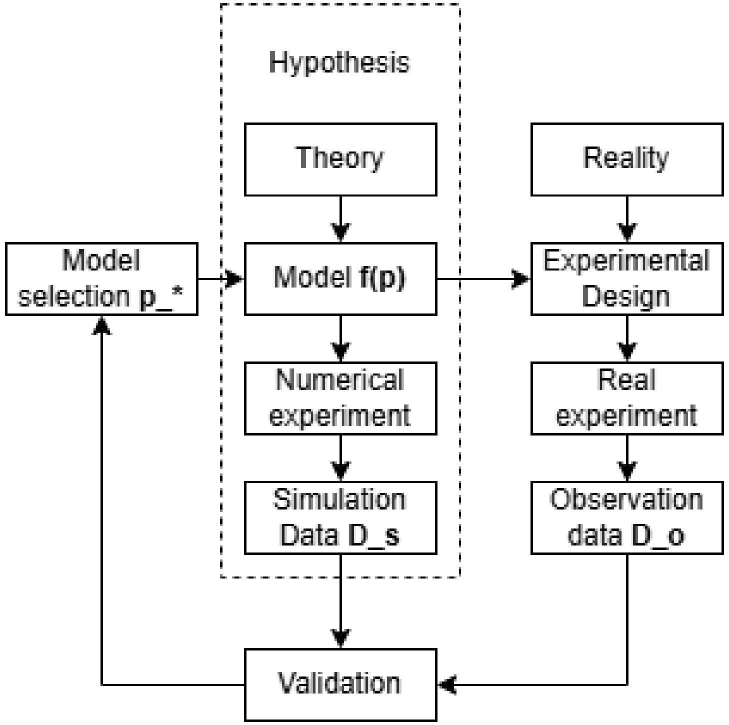
- Prior × likelihood ÷ evidence → posterior
- $p(\theta|\Theta, \mathrm{M}, \mathrm{D}) \propto \mathrm{L}(\theta|\Theta, \mathrm{M}, \mathrm{D}) \cdot \pi(\theta)$
- Markov Chain Monte Carlo

Moose STM:

- Likelihood: Gaussian
- Samplers: *IGMH, AISS, AID*

In wider sense:

- Selecting appropriate model
- Which model explains the data better?
  - What are model parameter values?
  - What physics need to be explained?
  - Which scales have to be resolved?



Intrusive Uncertainty Quantification: SFEM

Some properties *of Stochastic FEM (SFEM)* and *Stochastic Galerkin (SG)* methods

Advantages	Disadvantages
Highest accuracy available	New code development
Complex stochasticity treated in the same way as simple	Rigorous stochastic parameter specification – limited options
Solution yield all stat-s one can get with approximate PDFs	Know uncertainty on the phase of model construction
For many cases, most accuracy possible per unit of compute	Large coupled system to solve – can become too expensive
Parts (det. FEM blocks, PCE for stoch. terms) can be reused	Development difficulty increases quickly with new physics

TRIMAX – Tritium Reaction Integrated Multiphysics Analysis eXperiment

Digital Twin

- A bespoke predictive code for the experiment, which will develop into an operating code for LiBRTI experiments.
- General purpose companion for future experimentation which will inform design material and operating considerations for future reactors.

Uncertainty analysis

- Sensitivity Analysis methodology in support of design of experiments and future studies
- Uncertainty Quantification for rigorous experimental validation and potentially parameter inference and engineering tolerances estimates

Experimentation

- Provide archetypal system producing tritium under irradiation for digital twin validation.
- Further our understanding of the thermophysical properties of lithium ceramics.

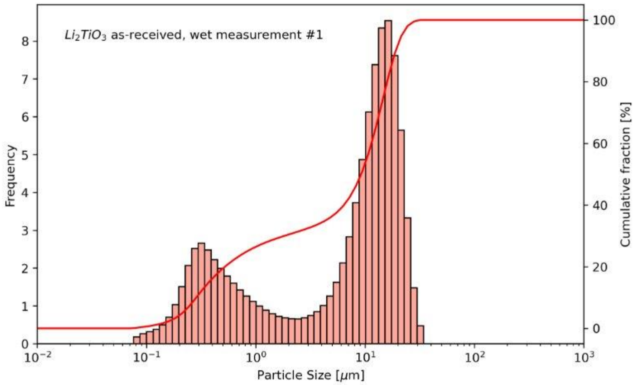
Thank you for your attention!

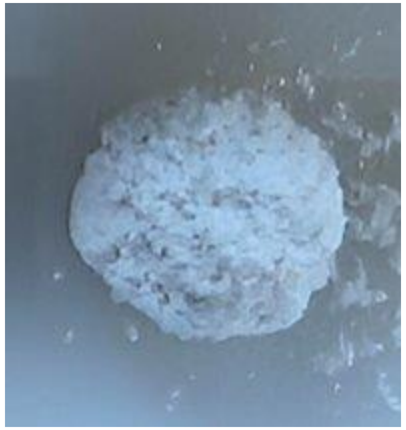
Back-up

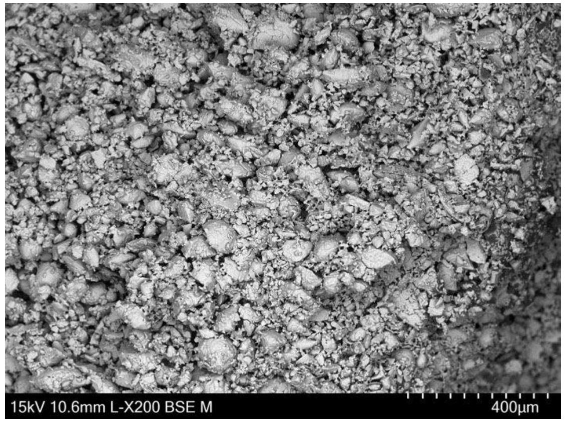
Lithium Ceramics: manufacturing

- Li_2TiO_3

- Binder jetting out of powder:
  - Initial constituent powder characterised
- Sintering:
  - Porosity analysed
- Production:
  - $\sim 10^4$ pieces possible







[By E. Zancan]

Updating Model: Behaviour

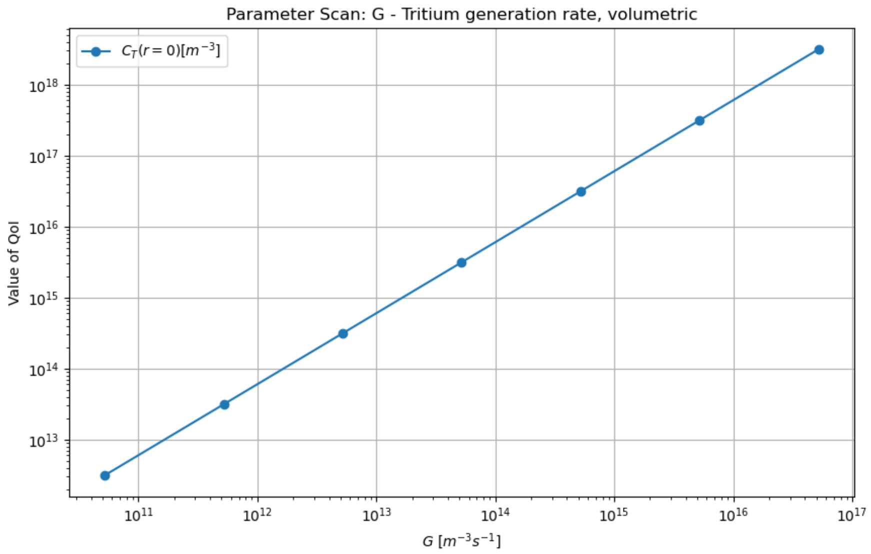
Dimensional Analysis & Empiric-numerical scaling:

Dimensionality: $C(r=0) \sim \frac{V\, G_T}{S\, J_T} \sim \frac{V\, G}{S\, D \nabla C} \sim \frac{R^3 G}{R^2 D\, \Delta C\, R^{-1}} \sim G\, D^{-1}\, R^2\, \Delta C$

Empirical: $C(r=0) \sim G\, D^{-1}\, R^2\, e^{-\alpha T}\, C_{BC}^{1/2}(r=R)$

Use as a $0D$ model to guide expectations:

- Auto-tuning solver parameters



Updating Model

- FESTIM 2.0.alpha8
- Gas and Heat transport:
  - Non-stationary diffusion in 1D spherical geometry

$$\frac{\partial C(r,t)}{\partial t} = D(T)\left(\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{2}{r}\frac{\partial C(r,t)}{\partial r}\right) + G(r,t)$$

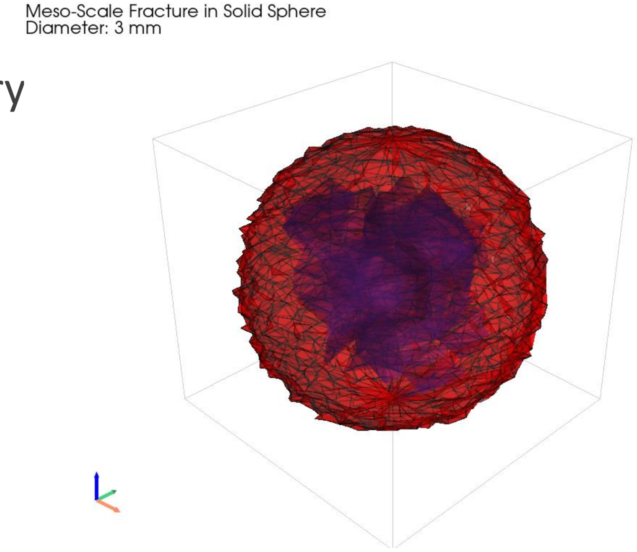
- Variety of BCs:
  - Surface reactions:

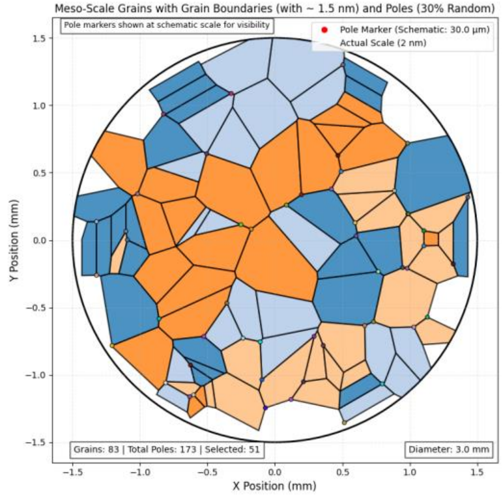
$$(-\nabla C_A \cdot \mathbf{n})\Big|_{r=R} = K = k_{r0} e^{-\frac{E_r}{k_B T}} C_A C_B - k_{d0} e^{-\frac{E_d}{k_B T}} P_C$$

  - Convective and radiative cooling:

$$(-\nabla T \cdot \mathbf{n})\Big|_{r=R} = h_{\text{conv}}(T_{\text{amb}} - T) + \epsilon\sigma(T_{\text{amb}}^4 - T^4)$$

- Suitable for grain or pebble –level modelling





3D grains, 3D surface, 2D grains – geometry by M.Mweetwa

Finite-volume model: spherical grain system

Physics:

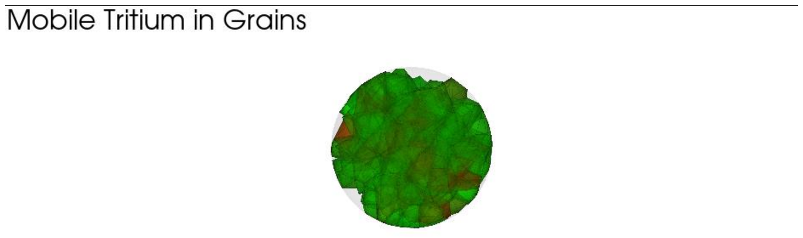
- Neutronics: experimental data
- Surface kinetics: MISTRAL
- Trapping
- Started: Helium Flow

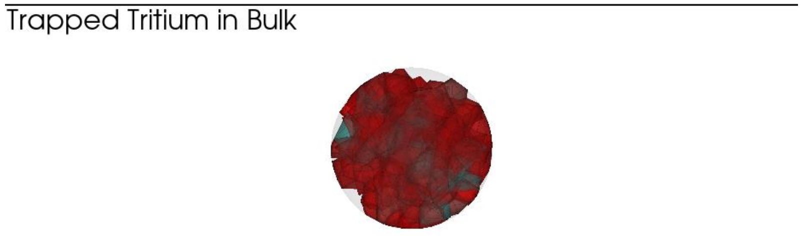
Geometry:

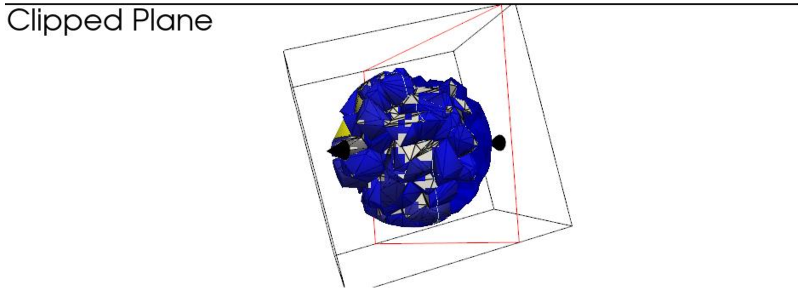
- Random network of spherical grains
- Inferred grain boundaries
- Variable number of grains

Numerical questions:

- Low single-grain resolution
- No grain geometry
- Conservation laws?







[By M. Mweetwa]

Uncertainty Quantification: Applied to the Model

- Parameters:
  - $G, Q, D, \kappa, h_{conv}, k_{r0}, k_{d0}$
  - Uniform, Normal
  - In terms of standard deviation, example: $\sigma = 0.05$
- Methods:
  - Polynomial Chaos Expansion (PCE)
  - Quasi- Monte Carlo (qMC)

$$Y \approx \hat{Y}(X) = \sum_{i=0}^{N} c_i P_i(X)$$

$$\mathbb{E}_{X\sim\mu}[f(X)] \approx S_n(f) = \frac{1}{n}\sum_{i=1}^{n} f(X^{(i)})$$

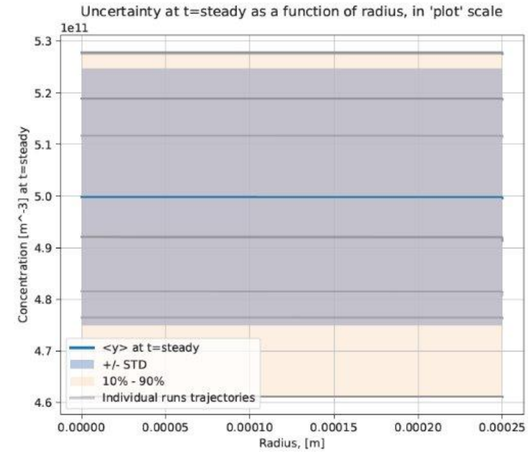
- Statistics:
  - Variance / Standard Deviation, Quantiles, Confidence Intervals
  - Sobol indices: first-order, total-order, second-order (interactions)

$$S_i = \frac{\mathbb{V}[\mathbb{E}[Y|X_i]]}{\mathbb{V}[Y]} \qquad S_i^{\text{tot}} = 1 - \frac{\mathbb{V}[\mathbb{E}[Y|X_{I\setminus i}]]}{\mathbb{V}[Y]}$$

Uncertainty Quantification: different aspects

Refinement of stochastic parameter:

- PCE of higher order: with full order implementation $N_{eval} \sim p_{order}^{N_{par}}$
  6 param: $64 \rightarrow 729 \rightarrow 4096 \rightarrow \cdots$ runs
- Other methods - MC : more “random” – can use sample for other methods

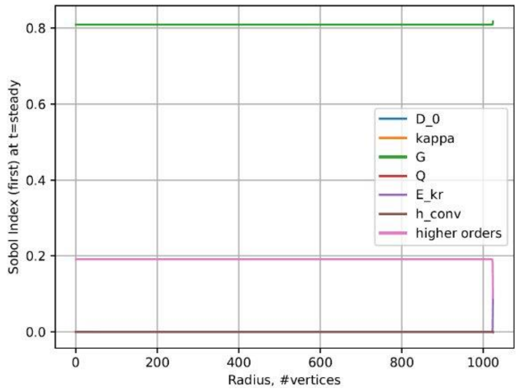


Parameter interaction:

- Second-order interactions can be non-zero

Different input parameter uncertainty specifications

- For toy problems – not very important, Example: Uniform error yield smaller variance than Normal ones
- Fitting complex statistic – might be more difficult



Uncertainty Quantification: Compute, Complexity, Timing

Timing:
- UQ campaign: $600\ [s]\ @\ 10\ CPUc$
- Code run, 1D: $0.1\ \left[\frac{CPUc \cdot s}{iterat.}\right]$

Complexity:
- Error $E = \|u - u_N\|_2$ reduction as a function of:
  - # uncertain parameters, uncertain parameter resolution, deterministic DoFs (problem size), time iterations,..

Method	# model evaluations	Average case	Best Case
PCE	$N_{eval} \sim \frac{(N_{par}+P_{pol})!}{N_{par}!P_{pol}!}$	$E \sim N_{eval}^{-r_{pce}}$	$E \sim A_{pce}^{-P_{pol}}$
MC	flexible	$E \sim N_{eval}^{-1/2}$	
SG		$E \sim A_{sg}^{-P_{exp}}$	

Uncertainty Quantification: Results

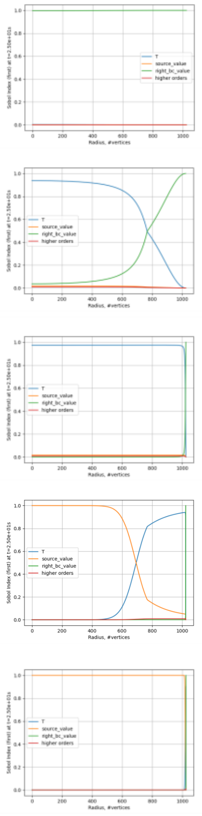
Some preliminary trends

- Uncertainty and sensitivities influenced by operation regimes
- Tritium generation is very important: neutronic uncertainty propagation
- Size of the grain and/or pebble is important
- Temperatures gradient are mostly weak
- Analysis of material data propagation and coupling smaller scales - WIP

Regime analysis: Sobol indices $S = S(r, \theta)$

- Domain (physical sample) size R_{max} : grain and pebble level
- Ambient temperature T_{amb}
- Tritium generation rate G

Automatic convergence test and rules



Uncertainty Quantification: correlated parameters

Problem expansion: coupled gas and heat transport

So far, one directional influence: heat → gas

Both are

- interdependent
- composition-dependant (cofounder)
- on atomistic level, have common/dependent channels

1. Study if coupling equations influence overall behaviour
2. How correlated parameters can influence behaviour
   - Potential dimensionality reduction
   - Account for more realistic physics

Uncertainty Quantification: correlated parameters

Approach:

1. NIUQ:

- A set of n correlated parameters $X_1, \dots, X_N$ described via covariance matrix K: $K = \left(\mathrm{Cov}[X_i, X_j]\right)_{i,j=1..N}$
- Decomposition/diagonalisation of K
  - Cholesky decomposition: $K = LL^T$
  - Rosenblatt transformation

$$F_i(x_i = s | x_1, \dots, x_{i-1}) = \frac{\int_{-\infty}^{s} f_{X_i}(x_1, \dots, x_{i-1}, s) ds}{f_{X_{i-1}}(x_1, \cdots, x_{i-1})} = \frac{\int_{-\infty}^{s} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_{X_i}(x_1, \dots, x_{i-1}, s) dx_1 \dots dx_{i-1} ds}{\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_{X_i}(x_1, \dots, x_{i-1}) dx_1 \dots dx_{i-1}}$$

- Full Sensitivity Analysis in terms of Sobol indices requires n cyclical permutations of original uncertain parameters

- Method and functionality existing, requires testing, defining data and regimes

Intrusive Uncertainty Quantification

Stochastic Finite Element Method:

- Treat Trial functions (to find solution) as random ones
- Expand stochastic term into series, as the first step of modelling
- Additional discretisation in probability space
- Larger problem, tensor product structure

Stochastic Galerkin:

- Construct basis via Galerkin projection:
- Error is orthogonal (in the selected trial function space $v \in V$) to the solution
  - Optimal, in some sense → in which case we should use it?

Intrusive Uncertainty Quantification: SFEM

- Express uncertain parameters via expansion:
  - Define appropriate basis – for output and random term
  - Truncate, up to P_u, P_A terms
  - Example: Gaussian Field → Karhunen–Loève Expansion (KLE):
- Define (stochastic) basis for problem and solution: e.g. PCE
- According to expansion, define a set of deterministic problems (size N)
- and assemble into large stochastic problem of size $N \times L$

$$\alpha(\mathbf{x}, t, \omega) = \mathbb{E}[\alpha(\mathbf{x}, t, \omega)] + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \xi_i(\omega) \psi_i(\mathbf{x}, t)$$

$$\int_D K(\mathbf{x}, \mathbf{y}) \xi_n(\mathbf{y}) d\mathbf{y} = \lambda_n \xi_n(\mathbf{x})$$

$$\mathbf{A}(\omega)\mathbf{u}(\omega) = \mathbf{f}$$

$$\forall k \in \mathbb{P}_u : \sum_{j=0}^{P_u} \sum_{i=0}^{P_A} \langle \xi_i \xi_j \xi_k \rangle \hat{\mathbf{A}}_i \hat{\mathbf{u}}_j = \langle \mathbf{f} \xi_k \rangle$$

→ Working a solution on base of *DOLFINX* and *ChaosPy*

Intrusive UQ: Stochastic FEM

Idea:

- Some parameters are closed-form stochastic processes/fields: $a(\boldsymbol{x}, \omega)$
- Stochastic parameters have decomposition in terms of random variables: $a(\boldsymbol{x}, \omega) = a_o(\boldsymbol{x}) + \sum_{m=1}^{\infty} a_m(\boldsymbol{x})\xi_m(\omega)$
- Solution is expressed in terms of physical $\phi(\boldsymbol{x})$ and stochastic basis $\psi(\omega)$
- Basis are functions of physical coordinate $\boldsymbol{x} \in D$ and possible quantity value at this point $\omega \in \Omega$
- Resulting formulation – double integral equation: … $= \iint_{D,\Omega} \ldots \cdot v(\boldsymbol{x}) d\boldsymbol{x}\, dp(\omega)$
- Resulting linear system after discretisation – tensor product: $\boldsymbol{A} = \sum_{m=0}^{M} \boldsymbol{G}_m \otimes \boldsymbol{K}_m$
- Solution is a discretised stochastic process – double sum: $\hat{u}(\boldsymbol{x}, \omega) = \sum_{i \in I_D, j \in J_\Omega} u_{ij} \phi_i(\boldsymbol{x}) \psi_j(\omega)$

Going for HPC

Name	Institution		Status
Marvin	NFI (local)		…
Hawk	Supercomputer Wales		decommissioned
Falcon	Supercomputer Wales		not yet operational
ARCHER2	EPCC, National		MOOSE ✔ → TMAP8✔ ; docker(singularity): non-parallel but **HTC**
Apocrita	QMUL		(conda/docker/src-compiled): **job-array operational**

- Hardware + software stack
- Support: technical, admin
- (Single/multi) –node scaling
- UQ → HTC / Pilot Job / ?
- More capabilities → total compute available → total physics/information produced
- ***Some issues***: parallel preconditioners (MOOSE recommendation); multiple build problems, …

Model benchmarking

Codes:

- FESTIM
- TMAP8

Verification & Validation:

- FESTIM V&V book [1]
- TMAP(4,7,8) verification document [2]
- CIVET approach
- MES, MMS; experimental data

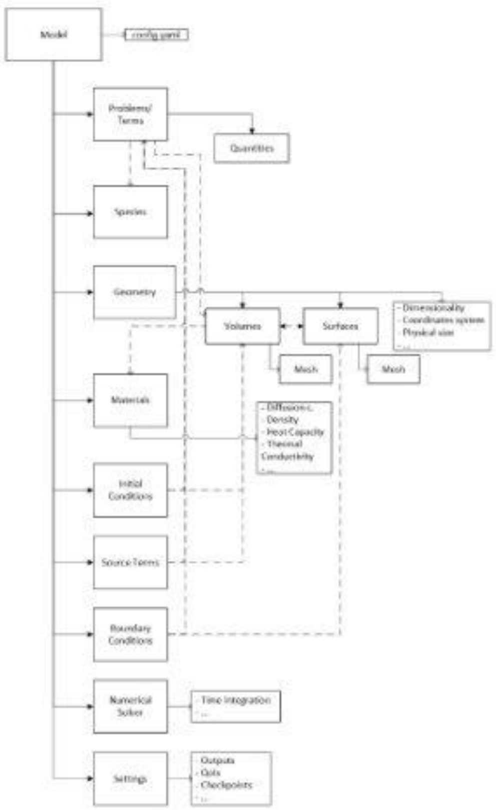
Benchmarking:

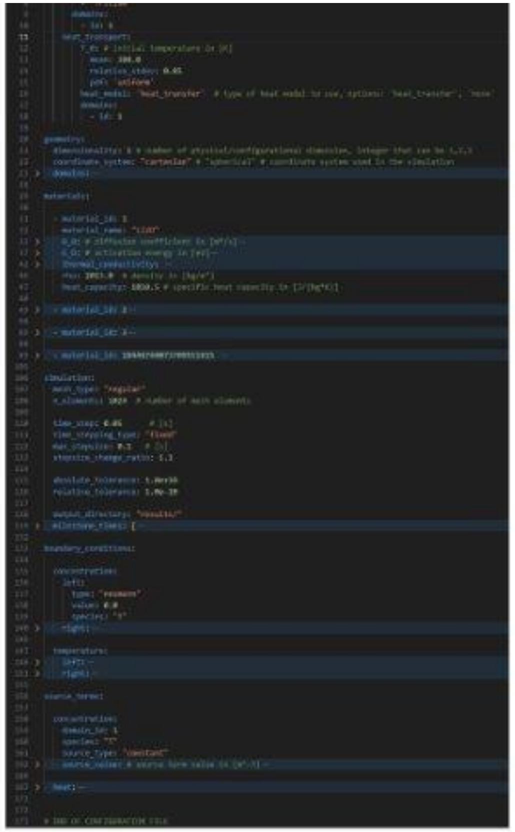
- Cases interesting for LIBRTI?
- Cases which include *UQ*?

[1] Remi Delaporte-Mathurin and Jair Santana, *FESTIM V&V Book*, 2024
[2] James Ambrosek. Verification and Validation of TMAP7. Technical Report INEEL/EXT-04-01657, Idaho National Lab

Updating Model: Software

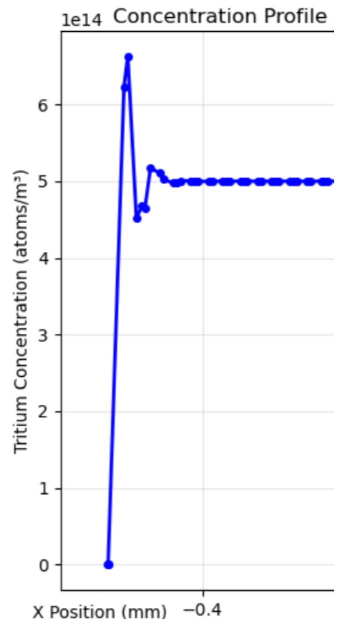
- YAML input configuration format:
  - Defines model schema
  - Parameter values and PDFs
- Model construction
  - Python OOP for FESTIM 1.4 & 2.0alpha
- Wrappers for scans
- “Encoders-decoder” for NIUQ
- Postprocessing:
  - QoI computation, visualisation





Updating Model: Issues

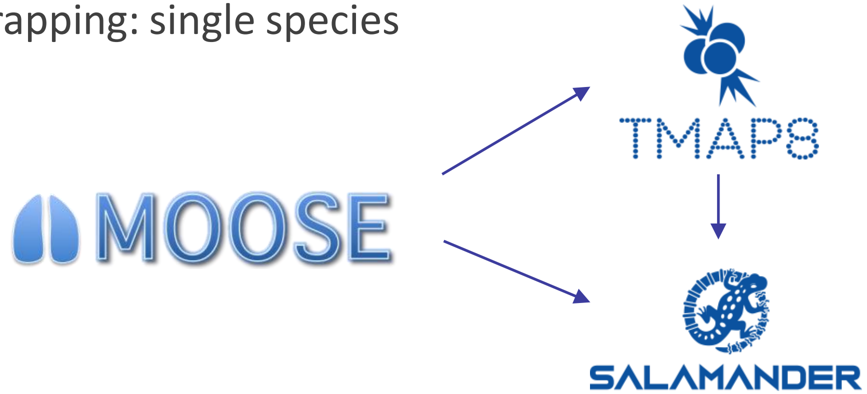
- PETSC SNES & KSP config:
  - Config heuristics – tolerances scales with solution for concentration
- Gibbs phenomenon:
  - Mesh refinement: linear regions, quadratic
  - Rules and implementation
- Multiple modes of failure discovered
  - Model updated
  - Solution for some numerical problems found
- In touch with developers



Gibbs phenomenon, discontinuity by FEM, – sim. by T.Griffith

TMAP8 based model

- Based on MOOSE
- SALAMANDER: coupling with neutronics via Cardinal: *OpenMC*
- Functionality:
  - 2D/3D
  - Domains with different phases (bulk/boundary)
  - Multi-species
  - Realistic sources (SALAMANDER coupling)
  - Boundary: recombination flux
  - Trapping: single species



- Methods to comply with numerics:
  - Solver tolerances: ✓..
  - Preconditioning: ***Issue for parallelism?!***
  - Mesh refinement: ✓..
  - Smoothing source etc. at boundary (polynomial decay): ***?***
  - Time-dependant BCs: ***?***
  - **Time-dependant source: ✓!**
- Interesting next steps:
  - Heat transport coupling
  - Realistic grain geometry: *PolycrystalVoronoi*
  - Realistic porous geometry: *ImageFunction* module
  - Coupling with atomistic scale effects
  - **3D+geometry+dimensions+params**
  - …

TMAP8 model scaling

Model configuration here:

- Boundary conditions (surface): recombination flux
- Source: constant
- Trapping & detrapping, no damage:
  - Single type
  - 2 Types: Li, Ti
- Geometry: grid-aligned crystalline & amorphous regions
  - 2D, square
  - 3D, cuboid

Runs:

- Apocrita @ QMUL
- SGE job array of *serial* jobs
- Linear scale for energies: $50 \ldots 150\%$
- Log-scale for flux and fraction: 2^n
- Cases:
  - 16
  - 4
- $t_{max}\ [s] =$
  - $1.5 \cdot 10^4$
  - $9 \cdot 10^2$
- $N_{DoFs} =$
  - 104802
  - 5184

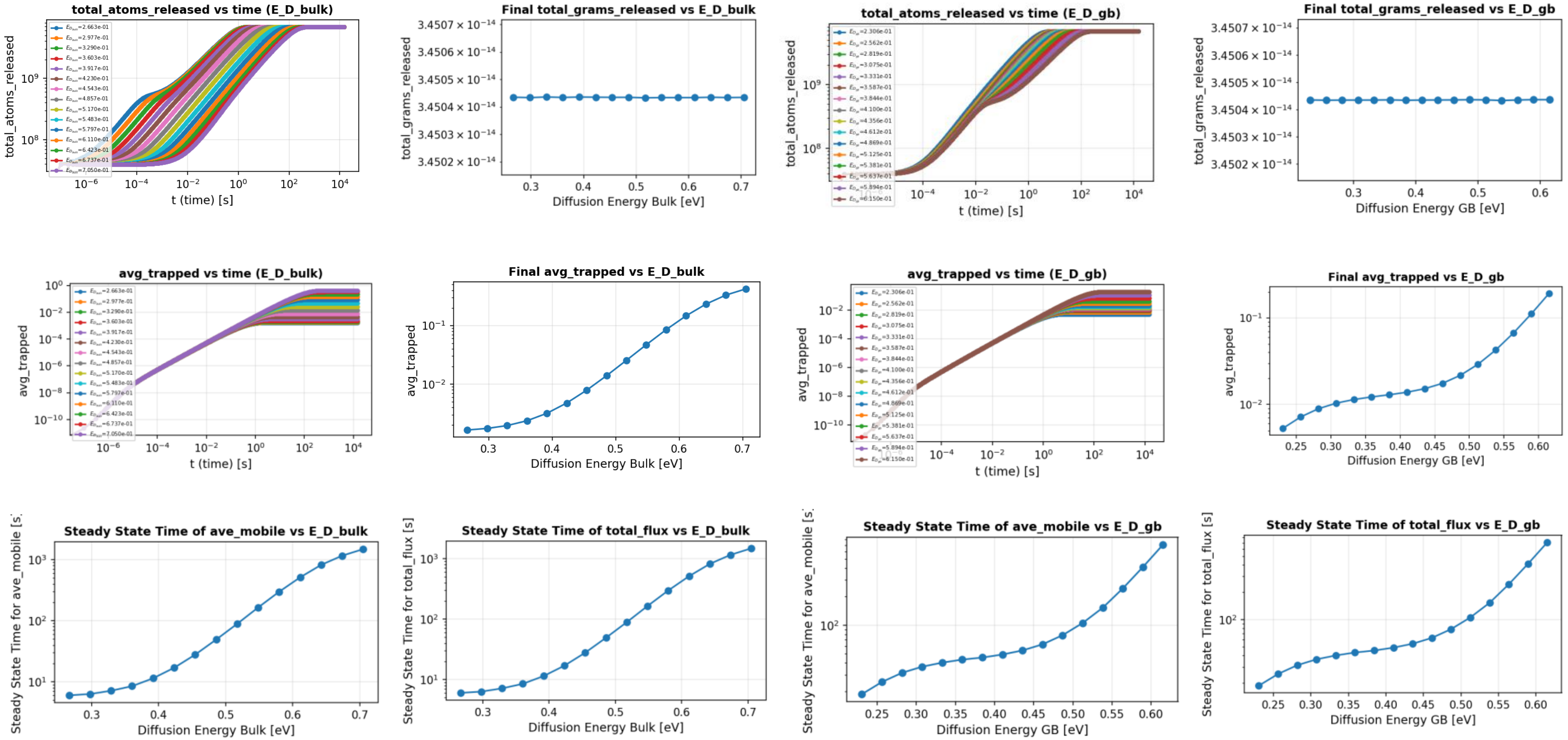
TMAP8 model scaling: activation energies – trapping, release, timescales

Total quantity vs t | Total quantity vs param. val. | Total quantity vs t | Total quantity vs param. val.

Total Release vs Activation energy

Total Trapping vs Activation energy

Time until steady state vs Activation energy



Crystaline bulk | Amorphous grain boundary

Timescale:

dependent on E_D^{bulk}, $E_D^{g.b.}$

steady state in $t \approx 5 - 500\ [s]$ approx.

$E_D^{bulk}: +0.1[eV] \rightarrow t_{s.s.}[s]: \times\ 10$

$E_D^{g.b.}:\ +0.3[eV] \rightarrow t_{s.s.}[s]: \times\ 10$

Trapping:

$\log \mathrm{N_{tr}} \sim E_D^{bulk}$

$\log \mathrm{N_{tr}} \sim E_D^{gr.b.}$

$E_D^{bulk}:\ +0.3[eV] \rightarrow N_{tr}[at.]: \times\ 10$

$E_D^{g.b.}:\ +0.3[eV] \rightarrow N_{tr}[at.]: \times\ 10$

Release:

$\mathrm{m_{T-r}} \sim \boldsymbol{const}$

functional forms?

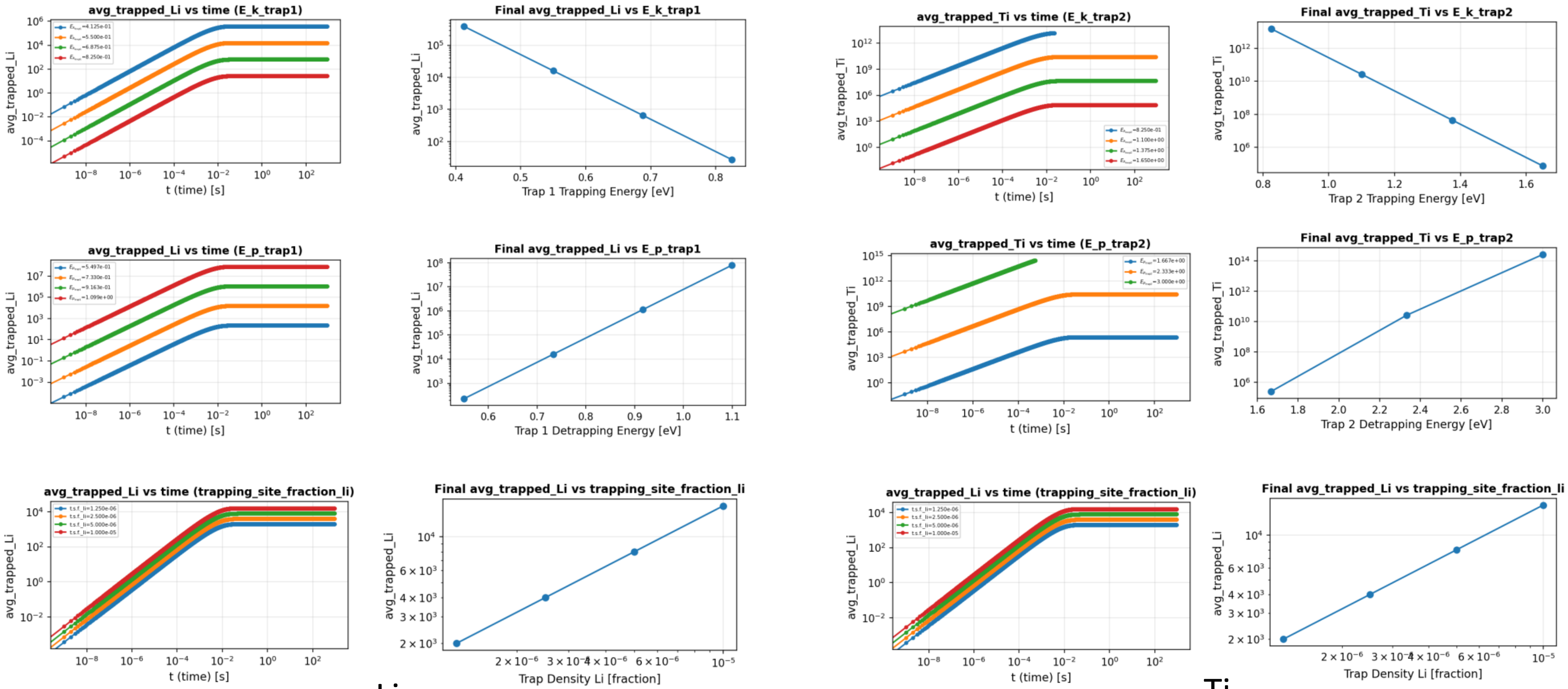
TMAP8 model scaling: Li & Ti trapping / de-trapping energies, trapping sites

Tot. trapped vs t | Tot. trapped vs value | Tot. trapped vs t | Tot. trapped vs value

Trap. energy

De-trap. energy

Site fr.



Li

Ti

Timescale:
steady state in $t \approx 1[s]$
(almost no dependency)

Trapping / Detrapping:
$\ln \mathrm{N_{tr}} \approx -23\, E_{tr}$
$\ln \mathrm{N_{tr}} \approx 23\, E_{dtr}$
$(\pm 0.1[eV] \rightarrow \times\, 10)$

$\mathrm{N_{tr}} \approx \boldsymbol{t.s.f}.$

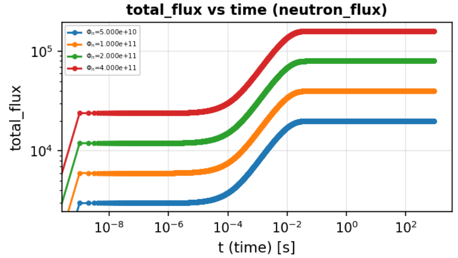
Sensitivities + interactions?

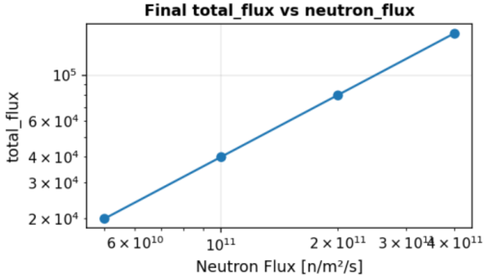
TMAP8 model scaling: neutron flux source - release

Tritium released vs t

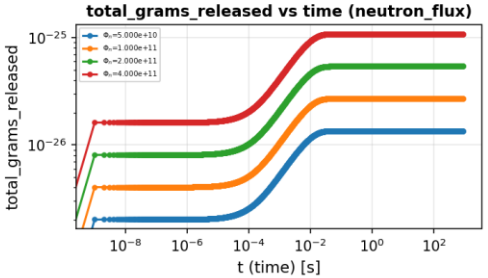
Tritium released vs value

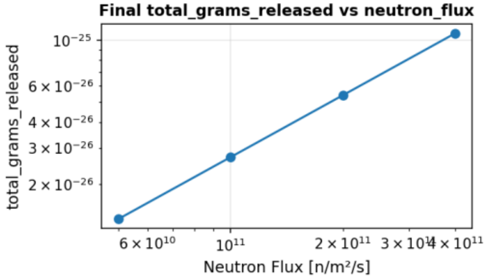
Neutron flux → Tritium atoms per s



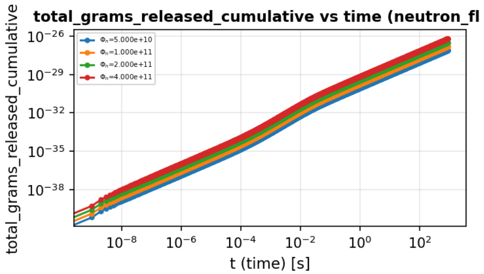


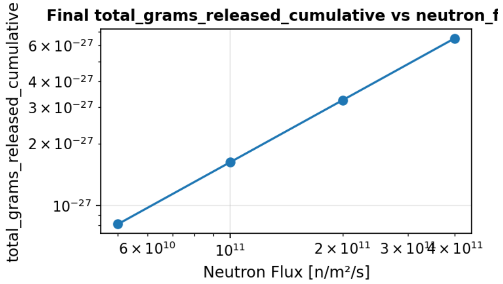
Neutron flux → Tritium grams per s





Neutron flux → Tritium atoms total





Timescale:

steady state in $t \approx 1[s]$
(almost no dependency)

Released Tritium:

$N_{T-r}, m_{T-r} \sim \Phi_n$

Cumulative Released Tritium:

$m^{tot}_{T-r} = \int_{t_0}^{t} m_{T-r}(t)\, dt \sim \Phi_n \cdot t$
(dynamics fast enough for initial stage not to matter)

Higher fidelity?
Interactions?
Correlations?

TRIMAX – Tritium Reaction Integrated Multiphysics Analysis eXperiment

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Digital Twin

- Predict breeder blanket outputs as a function of operation variables.
- Establish macroscale processes governing component performance and ageing.

Uncertainty analysis

- Fully specify uncertainty and safety margins under component operating conditions.
- Identify variables and processes chiefly responsible for final performance and stability.

Atomistic modelling

- Complement experimental data with predictions of physical parameters.
- Gain insight into microscale processes governing tritium mobility and retention.

Experimentation

- Provide archetypal system producing tritium under irradiation for digital twin validation.
- Further our understanding of the thermophysical properties of lithium ceramics.

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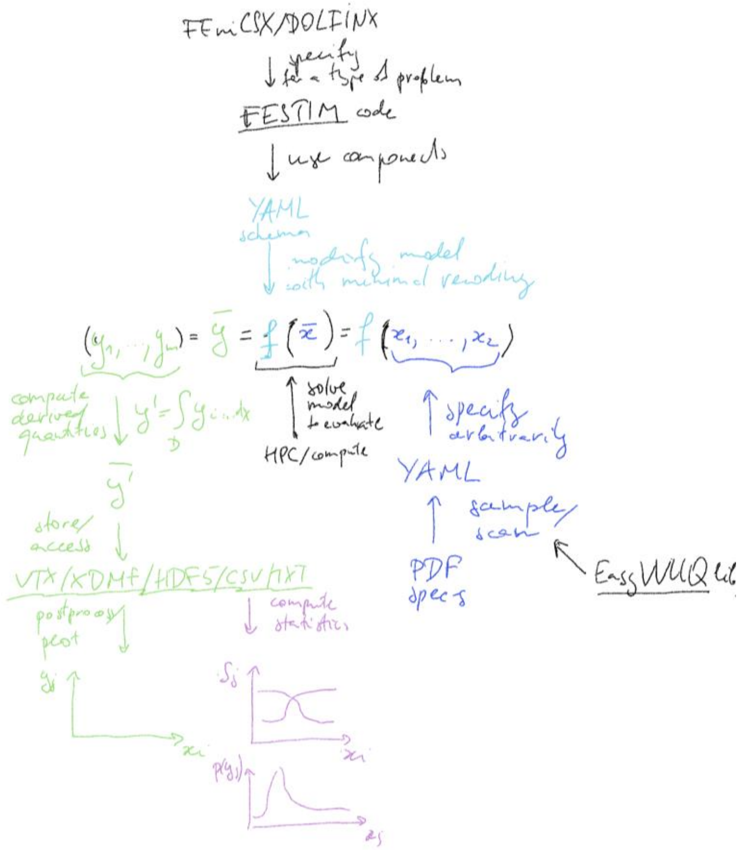
PI Cillian Cockrell; co-I Tessa Davey; co-I Simon Middleburgh

co-I Yu-Lung Chiu; co-I Enrique Jimenez-Melero

UNIVERSITY OF BIRMINGHAM

SW required for (NI)UQ



Directions to develop model