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An Integrated Multi-physics Platform for the LIBRTI Facility

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Workshop on Digital Engineering for Fusion Energy Research
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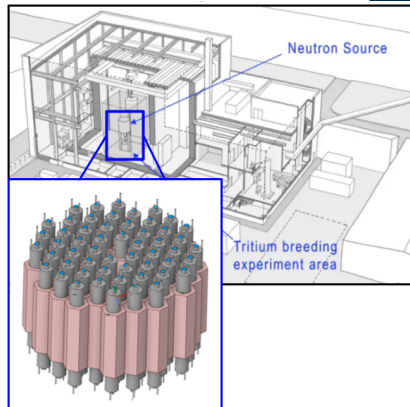
1. Introduction to LIBRTI Integrated Modelling Workstream
2. Recent Developments
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1. Introduction to LIBRTI Integrated Modelling Workstream

The LIBRTI Facility and Its Digital Replica

- **LIBRTI** (Lithium BReeding Tritium Innovation): planned UKAEA facility to test tritium breeding technology and validate modelling
- Compact **14 MeV** SHINE neutron source
- **Modular** experimental set-up for testing multiple concepts.
- We are building an integrated modelling platform to enable digital replica of LIBRTI's breeding experiments:
 - Assess uncertainties and improve **confidence in component-scale multi-physics modelling**.
 - **De-risk in-silico design** of future blankets and accelerate delivery.



Conditions for Digital Twins

Tests for Grieves and Vickers' Digital Twin:

1. **Sensory:** The virtual system is indistinguishable from physical system if manipulated.
2. **Performance:** Any action applied to both physical and virtual should result in identical behaviour.
3. **Reflectivity:** Equivalent information of current state may be obtained from both physical and virtual system.

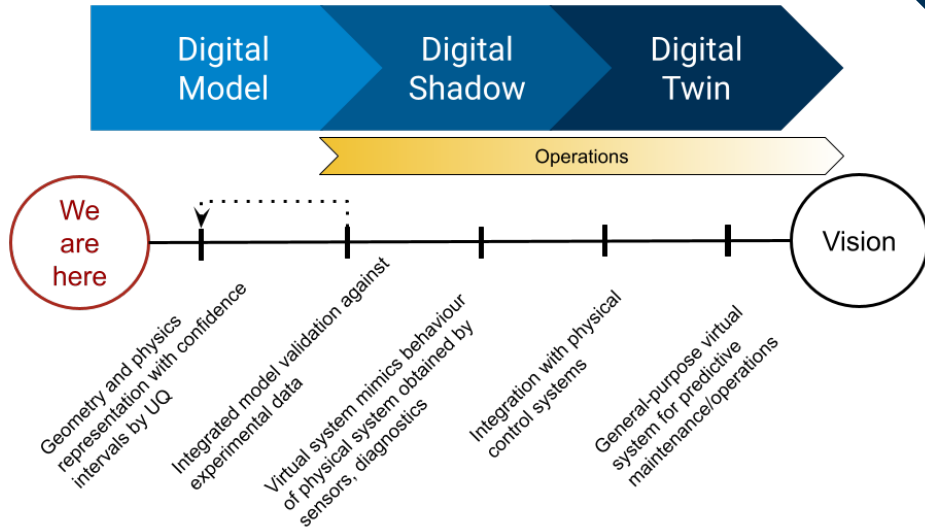
This enables:

- Avoiding unexpected, undesirable events - so called "black swans".
- Maximising desirable behaviour - through design, operations or maintenance.



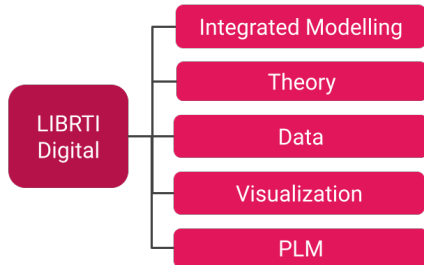
ChatGPT-generated image of a black swan carrying Grieves and Vickers' manuscript, "Digital Twin: Mitigating Unpredictable, Undesirable Emergent Behavior in Complex Systems".

Long-term Vision: From Models to Twins

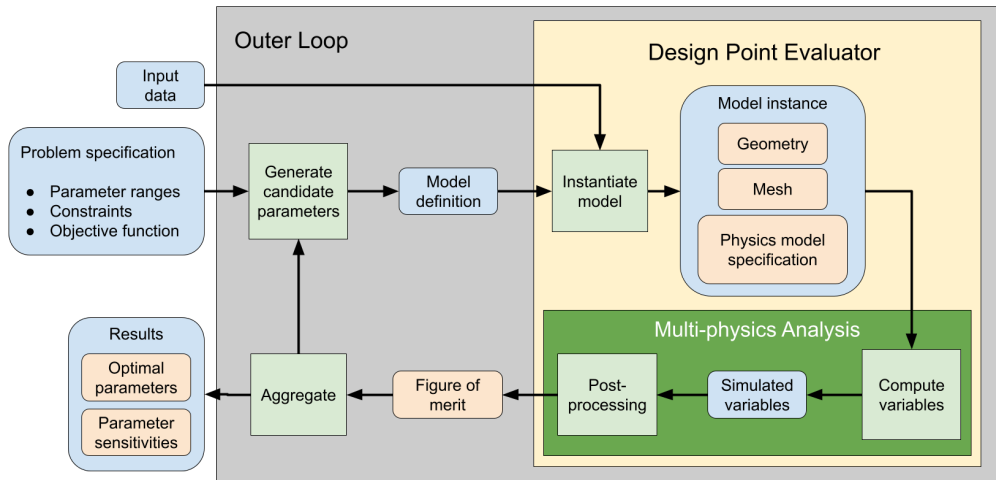


LIBRTI Integrated Modelling Activities

- Deliver a **flexible**, **scalable** and **portable** software solution to perform **multi-physics** simulation.
- Develop **high-fidelity models** of molten salt, solid and liquid metal breeder concepts.
- Develop **workflows** for **uncertainty quantification** and design **optimisation**.
- Codify all computational workflows using orchestration software, and storing in a **registry** for **reproducibility**, **findability** and **interoperability**.
- Coordinate with other LIBRTI Digital workstreams to progress TRL of **Digital Twins**.



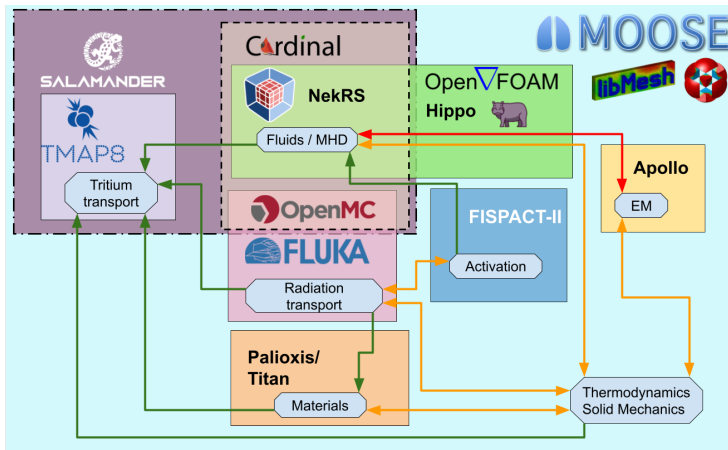
Idealised Digital Engineering Workflow

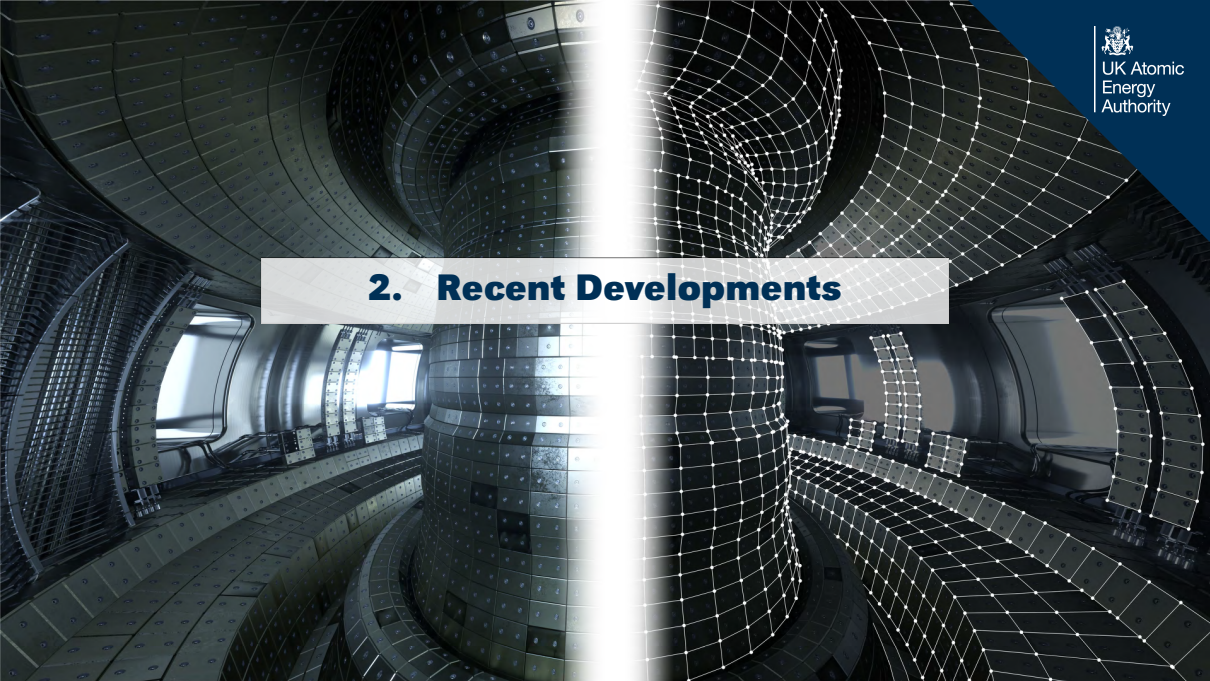


A Multi-physics Ecosystem for Integrated Modelling

See also talks by:

- Guillaume Giudicelli (MOOSE)
- Lane Carasik (Salamander)
- Casey Icenhour (Salamander)
- Alex Blair (MOOSE-MFEM)
- April Novak (Cardinal)
- Pierre-Clément Simon (Salamander)



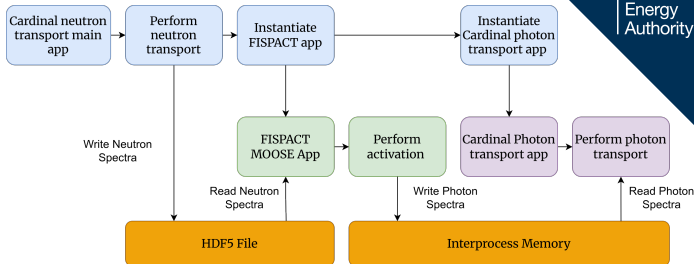


2. Recent Developments

FISPACT-II Integration with Cardinal

Purpose:

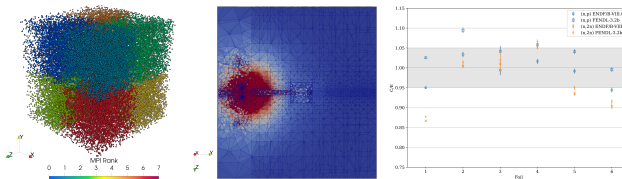
- Streamline shutdown dose rate calculations
- Fluid transport of activated materials
- Impact of decay heat



Current status:

- Workflow implemented
- Distributed photon source sampling is verified
- Validation against SINBAD FNG benchmark under way.

Data flow for shutdown dose rate calculation.



Distributed sampling visualisation (left) and preliminary validation results (centre, right).

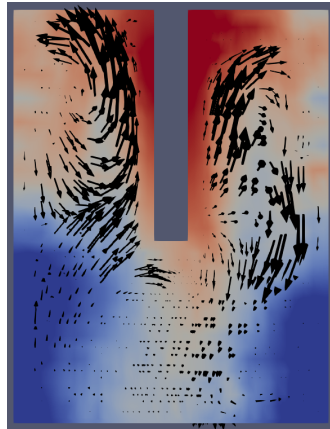
Credit: Bill Ellis

Molten Salt Breeder Modelling with Cardinal

Model advective transport of tritium using OpenMC for tritium production source, and NekRS for fluid velocity and conjugate heat transfer.

- Purpose:
 - Characterise spatial tritium distribution
 - Determine initial concentrations at salt / solid and salt / gas interfaces as precursor for permeation and extraction modelling
- Status: Proof of concept achieved for LIBRA geometry with an assumed temperature gradient.
- Next steps: Model thermal behaviour of BABY experiments; perform UQ + validation.

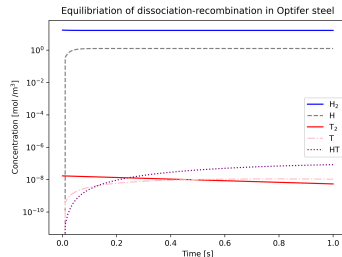
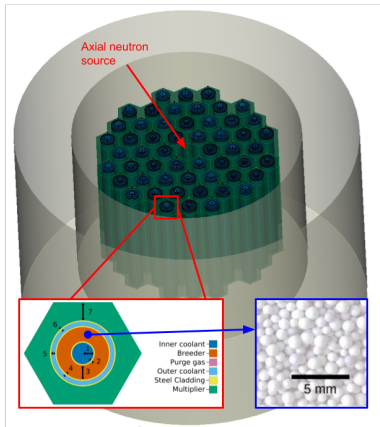
Credit: Sharp Lo



Solid Breeder Modelling with TMAP8 and Cardinal

Model diffusion-advection in porous medium with TMAP8; dissociation / recombination at interface.

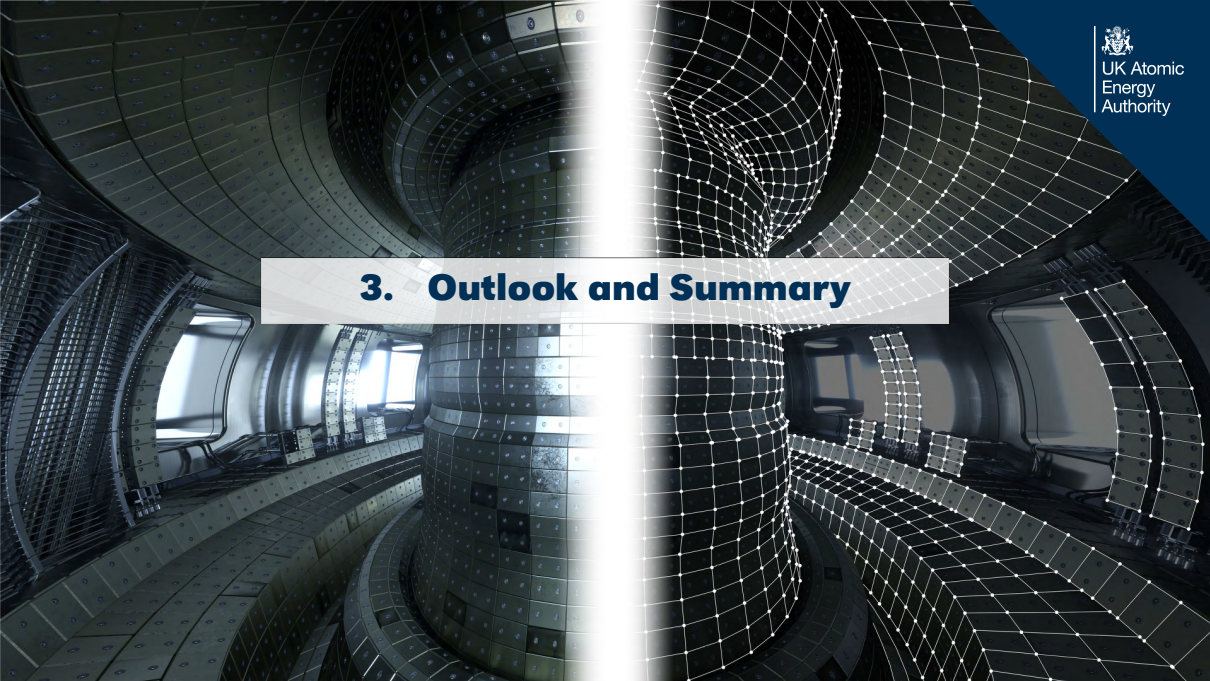
Preliminary findings indicate (for initial Hydrogen partial pressure of 2% = 1 bar) **majority of tritium exists as HT form.**



Next steps: unify modelling using Salamander (TMAP8 + Cardinal), perform UQ.
Credit: Sid Mungale

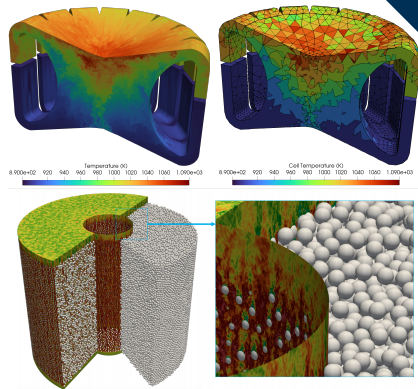
- See more: Humphrey et al (2025) *“Accelerating Engineering Design of Breeder Blankets with Parametric Optimisation and Sequential Learning”*, Frontiers in Nuclear Engineering





3. Outlook and Summary

- **Assess temperature dependence** in molten salts breeders + validation against experiment
- **Multi-phase flow** modelling of molten salt sparging + validation against experiment
- **Resolved flow** around pebble bed: assess impact of reduced-order thermal hydraulic correlations
- **Shutdown dose rate** of facility with FISPACT-II
- **Fluid Activation** with FISPACT-II + Cardinal
- **Neutron source modelling** with Fluka
- **Multi-scale modelling** of tritium transport parameters



*Examples of Cardinal modelling.
Top: pebble bed reactor, Fischer et al (2021).
Bottom: molten salt reactor, Novak et al. (2023)*

Workflow Orchestration

An extensive requirements capture exercise has been conducted.



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*"I am a scientist,
expected to exploit
simulation tools to
produce results and
studies for use in the
LIBRTI program"*

Work can be repeated,
reproduced and
validated. Business
decisions based on
simulation outputs can
be reviewed if inputs
change.

DATA-010:
Provision to record
sufficient workflow
metadata that any
workflow run can
be reproduced.

- **63 requirements** recorded, categorised with a rating:
"Must have" / "Should-have" / "Could have" / "Won't have"
- Priorities include: **usability, reproducibility, interoperability, scalability.**
- **Down-selection** of platform in currently under way.
- Future analyses (e.g. UQ campaigns, validation) will be **encoded** in the selected platform, stored in a registry and assigned a DOI - provides a **reference for PLM.**

Summary

- LIBRTI is a planned UKAEA facility to test **tritium breeding technology** and **validate component-scale modelling**.
- The LIBRTI Integrated Modelling workstream is delivering a flexible and scalable software solution for **high-fidelity multi-physics simulation**.
- Near-term outlook will focus on **increasing model confidence** through: verification, validation, uncertainty quantification, automation and reproducibility.
- Long-term outlook will seek to progress TRL towards a digital shadow or twin, enabling **risk-reduction** for in-silico design of blankets.

