amentum

Towards a Tritium Breeder Digital Twin

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Workshop on Digital Engineering for Fusion Energy Research
9th December 2025

AMENTUM PROPRIETARY

Agenda

1. Tritium Breeding and LIBRTI
2. Physics Simulation
3. Machine Learning Application
4. Software Infrastructure

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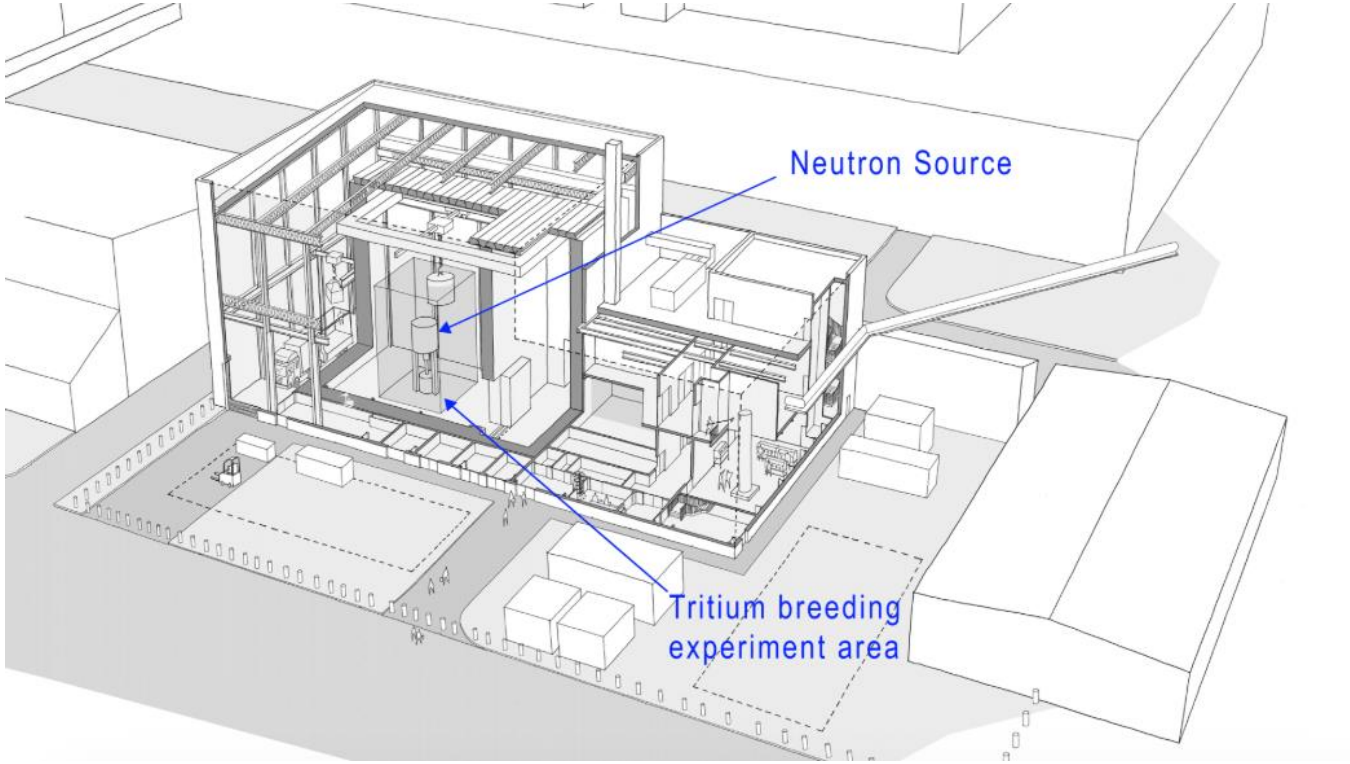
LIBRTI Programme

UK Atomic Energy Authority

- UKAEA £200 million investment 2023 – 2028
- Testbed facility for engineering-scale tritium breeder blankets
- To be build at Culham site (UKAEA)
- Commercial 14.1 MeV neutron source
- Pre- and post-experiment activities

- Flexible and scalable digital platform that enables full in-silico replication of breeding experiments
- Increased enablement of industry and academia to use LIBRTI
- Expand key UK skills through design, build and operation of a first of a kind facility, including within the supply chain



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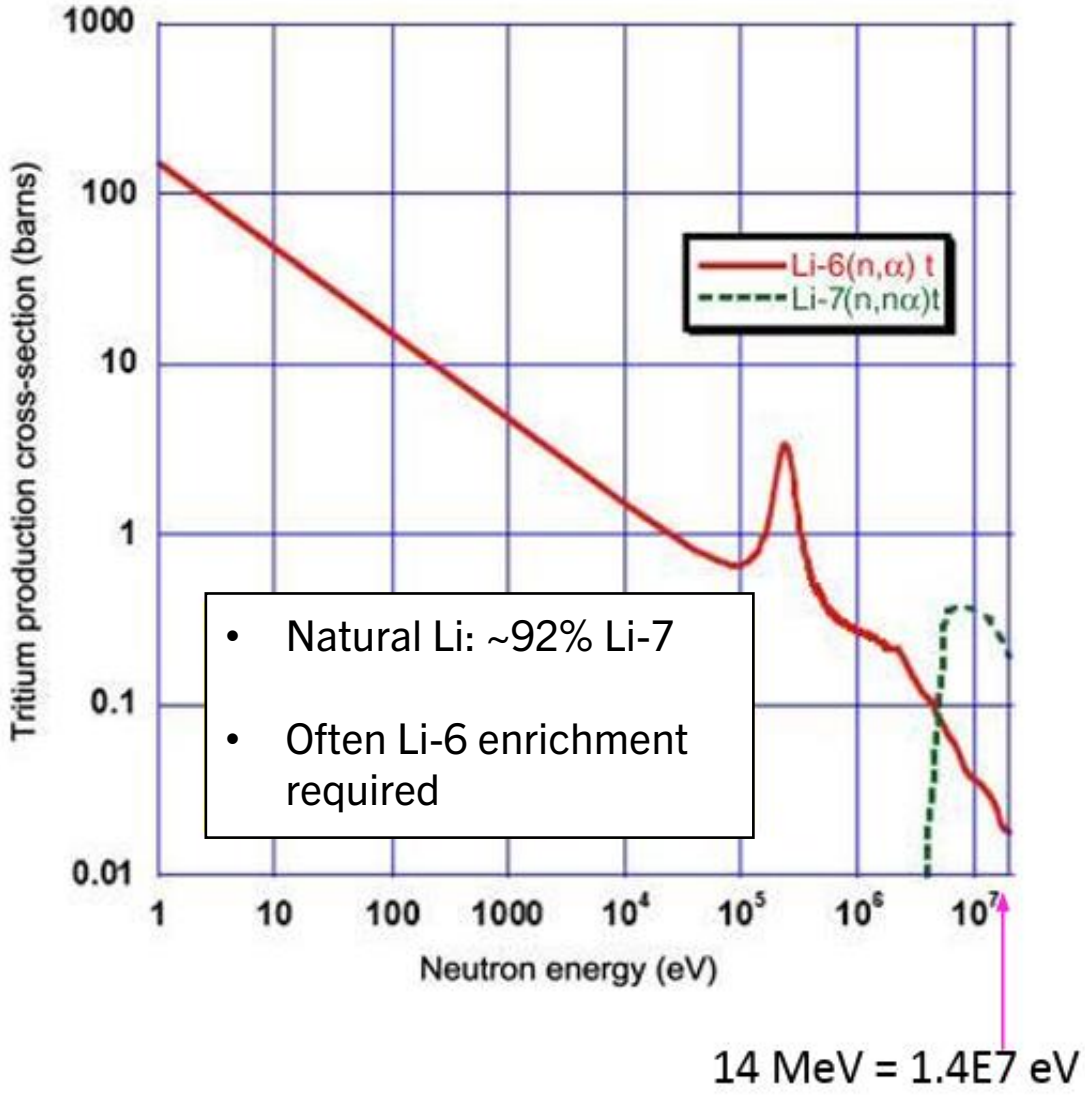
Tritium production

Lithium commonly used for tritium breeding due to its large reaction cross sections

- Li-7 + n -> T + He-4 + n'
- Li-6 + n -> T + He-4

Neutron multiplication (e.g. Be, Pb) used to boost tritium production:

- Be-9 + n -> 2 He-4 + 2n'
- Pb-208 + n -> Pb-207 + 2n'



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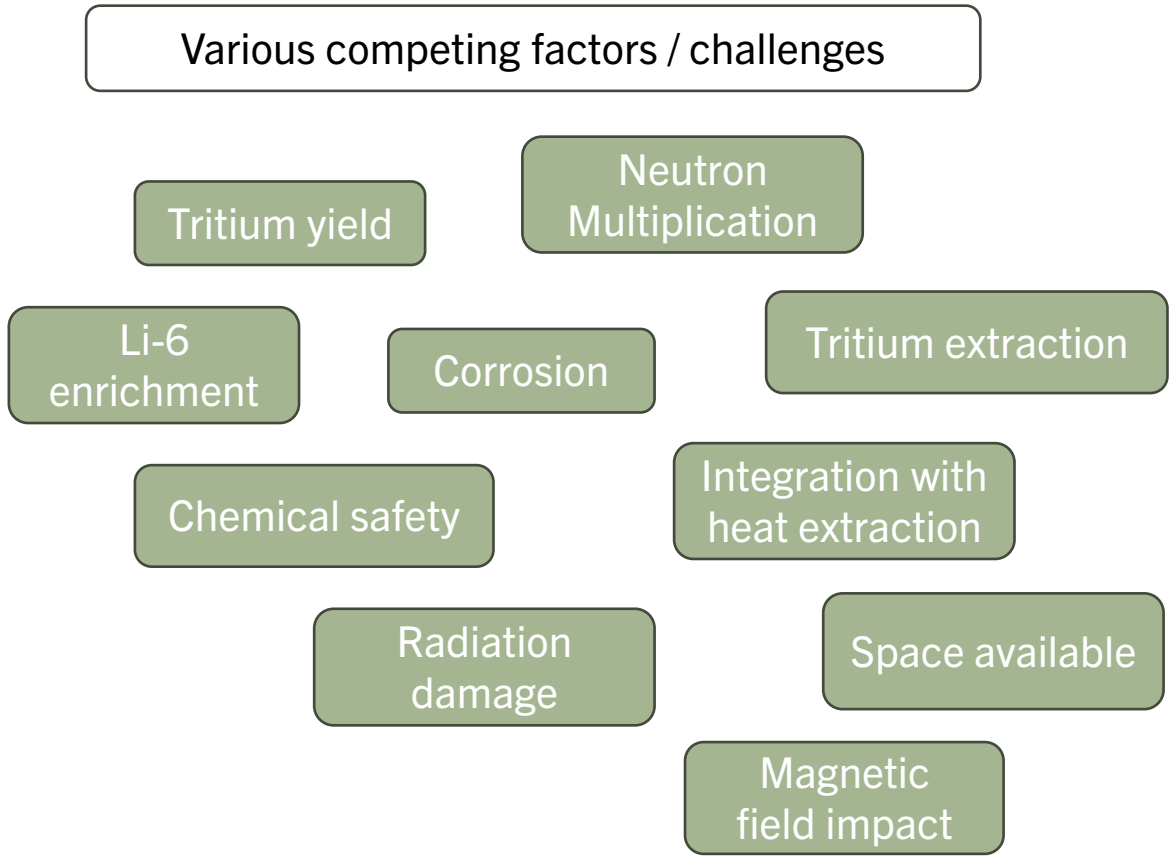
Towards a Liquid Lithium Breeder Digital Twin

UK Atomic Energy Authority

- Contract with UKAEA: development of Digital Twin for Liquid Lithium Breeder concepts at LIBRTI
- Main drivers:
  - Optimise breeder design
    - (e.g. tritium production / extraction, corrosion)
  - Optimise use of facility (experiment planning)
  - Predictive maintenance
  - Support decommissioning
- Approach:
  - Focus on most relevant (tritium rate)
  - Integrate DigiLab's Uncertainty Engine (ML and UQ)
  - Start before physical twin exists ('Digital Shadow')
  - Modular design / add phenomena as needed
  - Develop secure software infrastructure
  - Add feedback from physical twin



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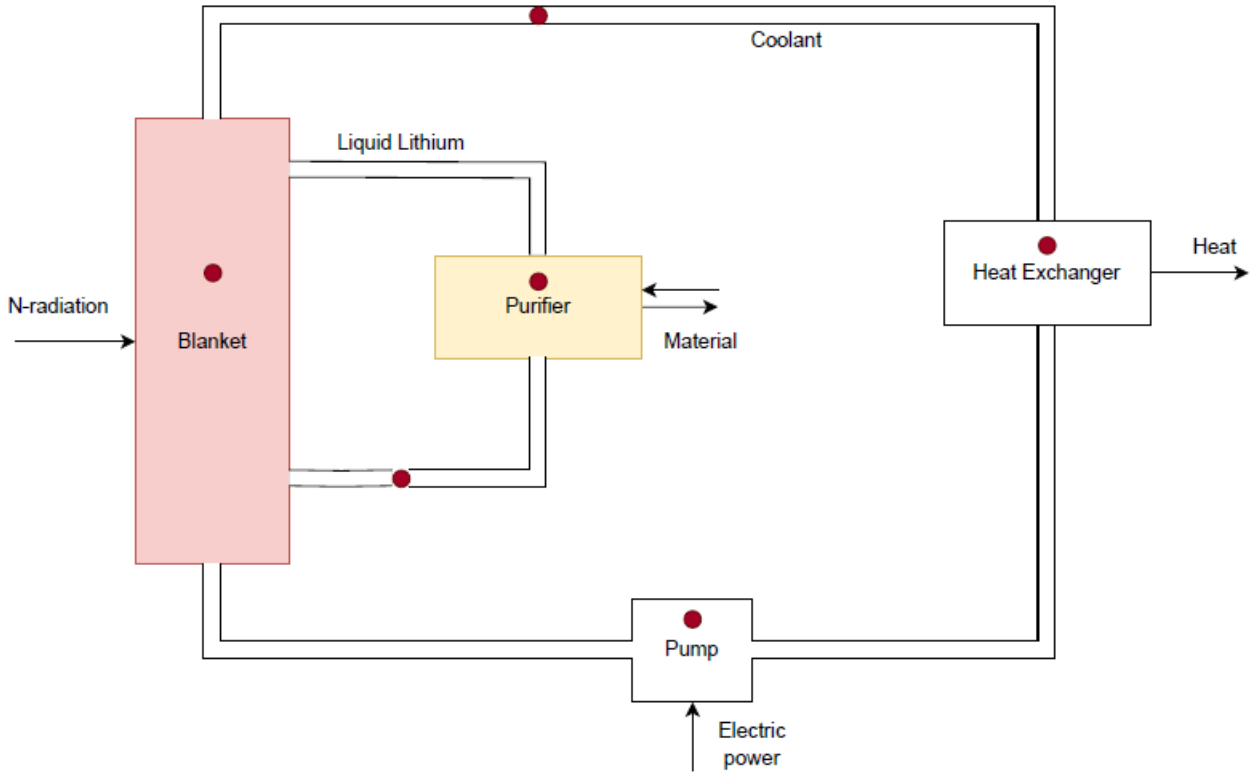
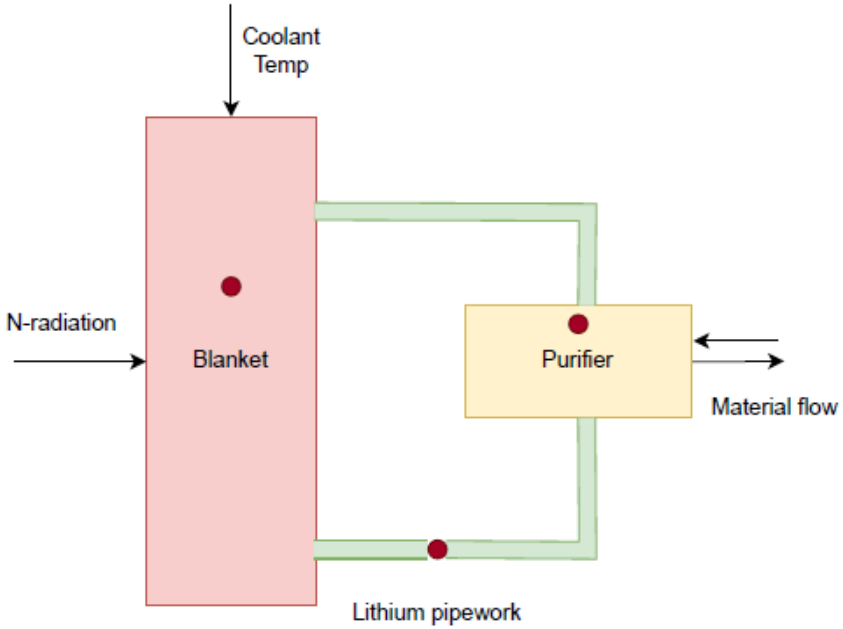
System Representation

General



Key physics:
- Neutronics, Activation
- Thermal-hydraulics
- Chemistry, Corrosion
- Material Loss

Initially considered



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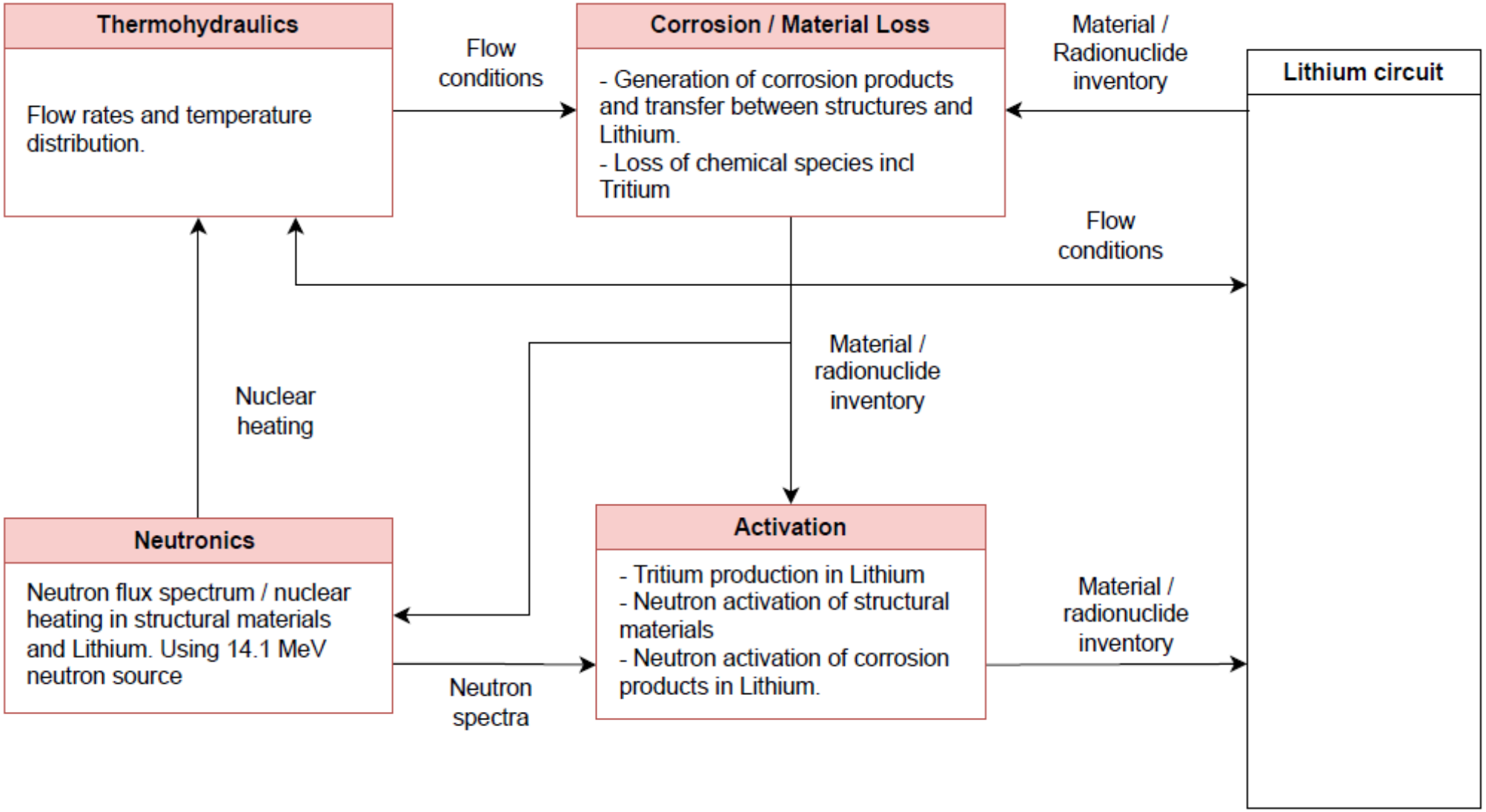
Physics - Blanket Node



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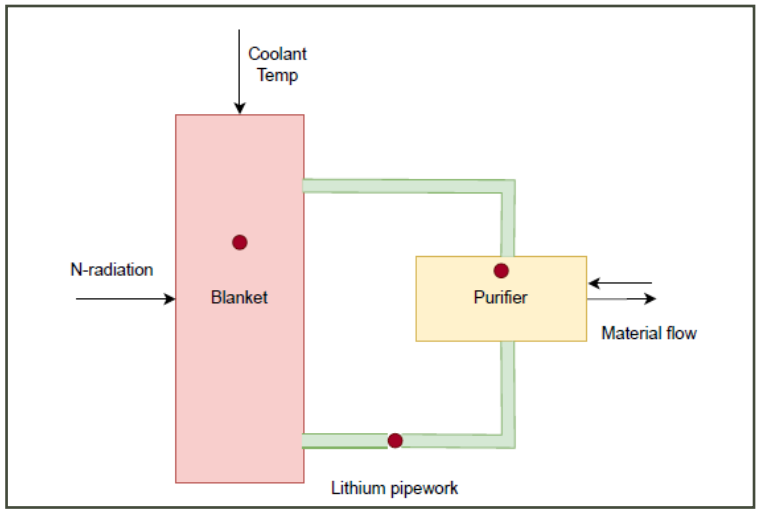
Initial Simulation Scope



Data

- Geometry
- Materials
- Fusion neutron source
- Flow rate, temperatures
- Purifier performance
- Corrosion rates
- Deposition / loss rates

Corrosion

Accumulation of corrosion products in Lithium.

Material Exchange / Decay (Purifier)

- Removal / addition of chem species
- Nuclear decay

Material / Radionuclide inventory

Material / Radionuclide inventory

Neutronics

Neutron flux spectrum in Lithium.
Using 14.1 MeV neutron source

Neutron spectra

Activation / Decay / Material Loss

- Tritium production in Lithium
- Neutron activation of corrosion products in Lithium
- Nuclear decay
- Loss of chemical species incl Tritium

Material / Radionuclide inventory

Material Loss / Decay (Pipework)

- Loss of chemical species incl Tritium
- Nuclear decay

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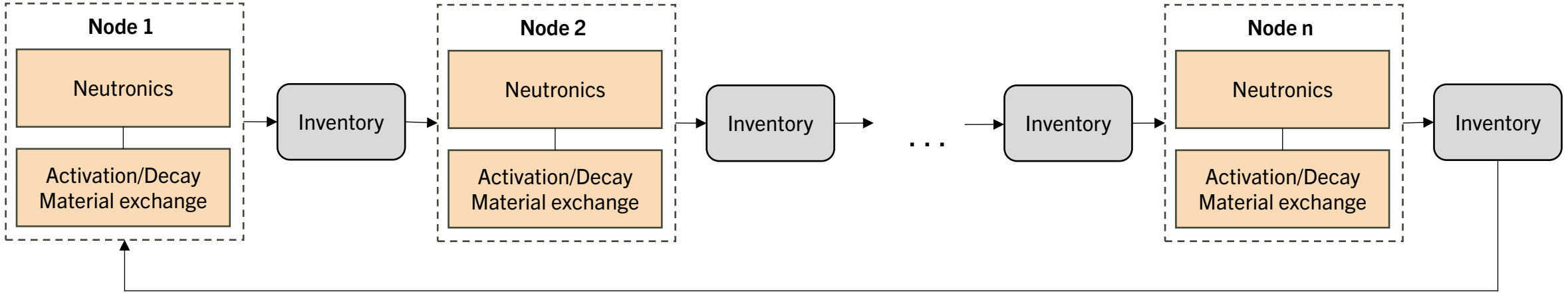
Generic System Model – Simulation Engine

- Nodes represent parts of Li circuit (e.g. blanket, piece of pipework)
- Simulation of relevant physics can be switched on/off for each node
- Able to model broad range of dynamic systems
- Time step based calculation

Initial Codes:
Neutronics: MCBEND®, part of
Amentum ANSWERS software suite:
https://www.answerssoftwareservice.com/
Activation/Decay: FISPACT-II
Material exchange: Analytic



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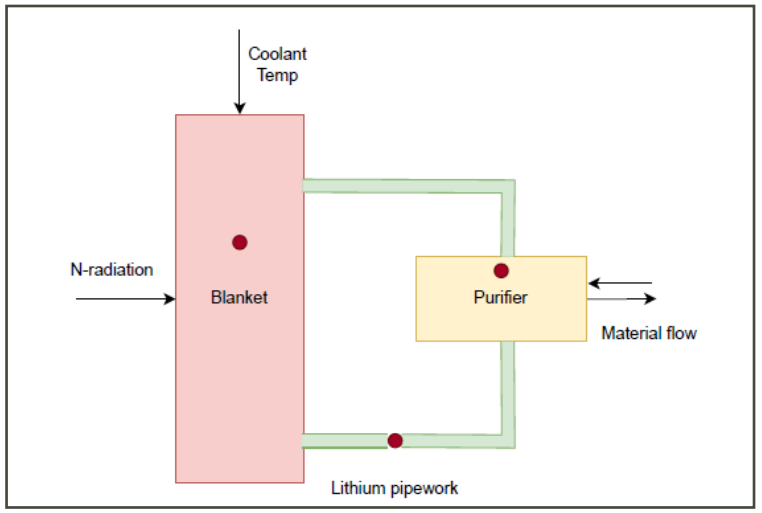
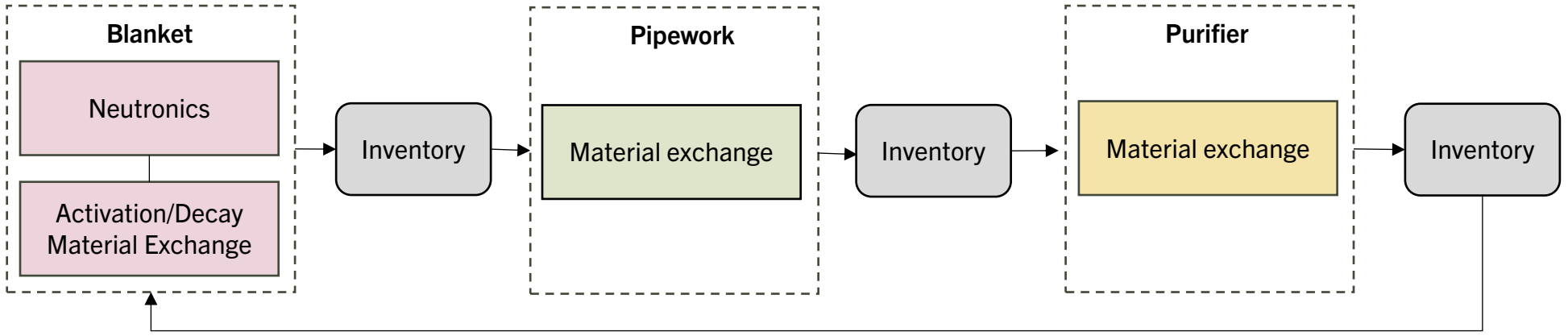
Example Configuration





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Model refinement

Neutronics Model	Activation Model	Purification Model	Corrosion Model	Thermohydr. Model
MCBEND 1D	FISPACT inventory	Equation based, const. rates	Experimental data / literature	Const temp/flow rate
MCBEND 3D	FISPACT inventory + radiolog. results	Equation based, time dependent	ML model	Equation based
MCBEND 3D + detailed source	FISPACT inventory + RANKERN dose rates	CFD + chemical		CFD

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Integration of Uncertainty Engine

digiLab

Uncertainty Engine by DigiLab:

- Trainable generic model, based on Gaussian Process approach
- Can be used to generate surrogate models to replace slow accurate models or when data is sparse
- Provides information on model uncertainty. This can be used to direct effort on obtaining additional data
- ML models run in cloud or locally

Areas of integration:

- Use of fast surrogate model for MCBEND® + FISPACT
  - Efficient sampling of design parameter space
  - Fast design optimisation
- Corrosion model: use of experimental data incl from Amentum's Liquid Lithium Test Facility

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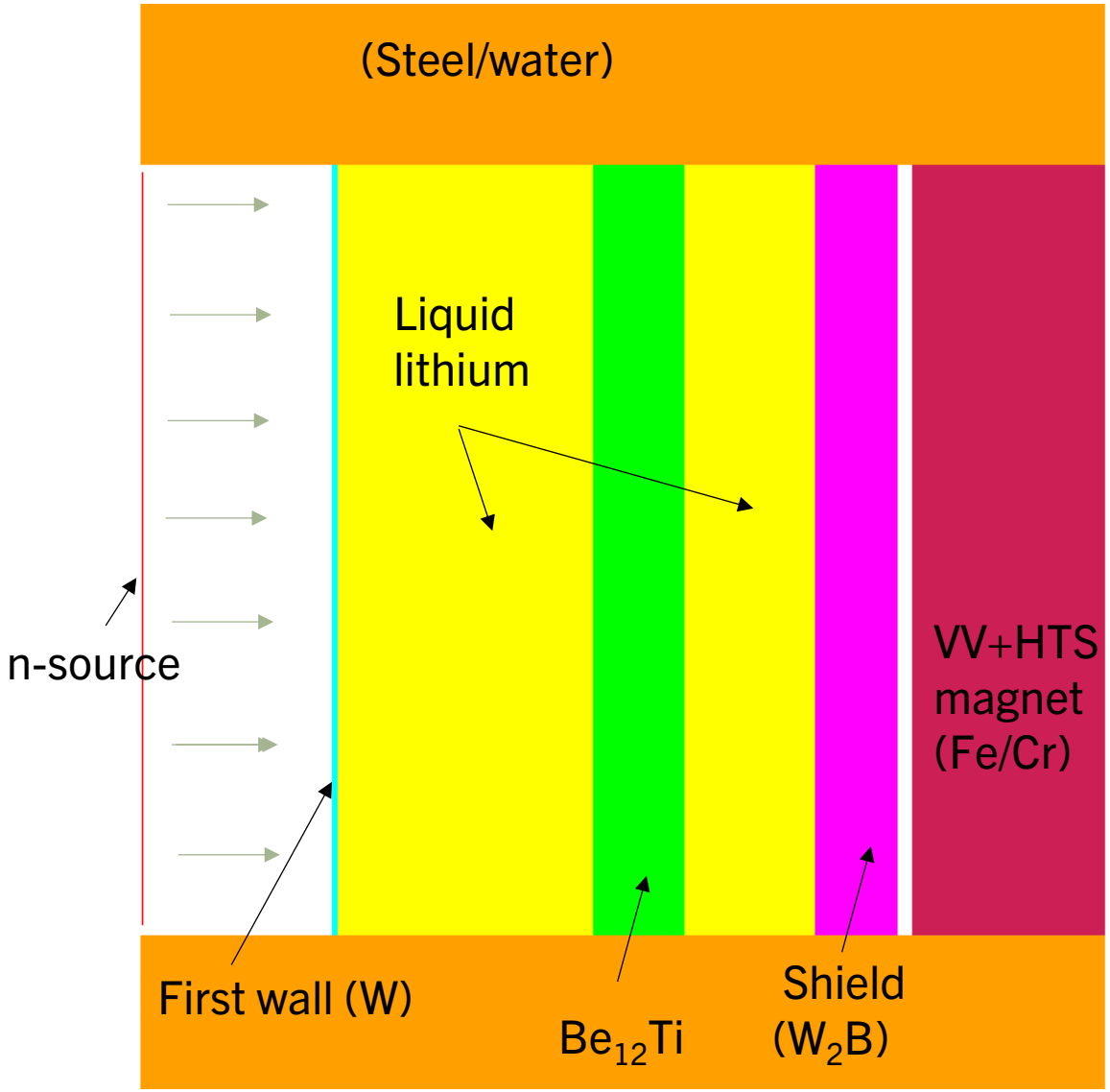
Example Breeder model

- MCBEND® model developed based on recent publication *
- Simple model for short run time
- Design complex enough to enable some design parameters
- Use for development of ML application



* Novel high temperature tritium blanket designs for confined spaces in spherical tokamak fusion reactors, M.D Anderton ,C. Baus, T.P. Davis, R.Pearson, K.Mukai, J. Pollard, K.Taylor, S.Kirk, J.Hagues, Fusion Engineering and Design 210 (2025) 114732

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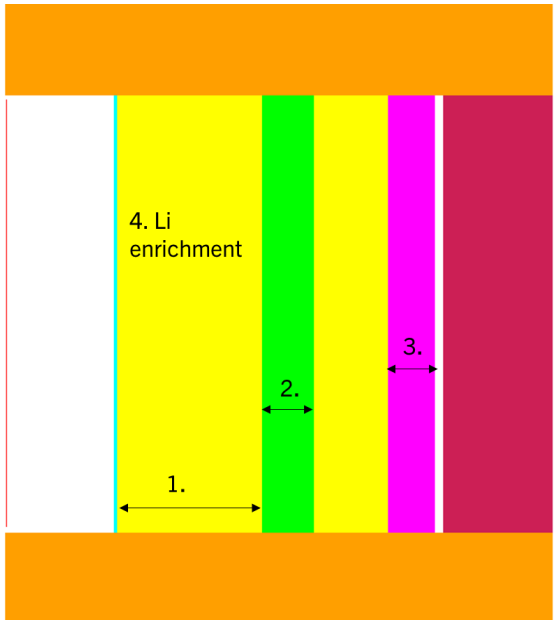
Setup without ML



Li1_th
BeTi_th
Shield_th
Li6_prop
…

MCBEND®

Neutron flux spectrum

Incoming Inventory:
Trit
He
Li6
Li7
…

Pipework

Blanket
(Fispact)

Inventories produced
at each time step

Outgoing Inventory:
Trit, He, Li6, Li7 ,…

Purifier

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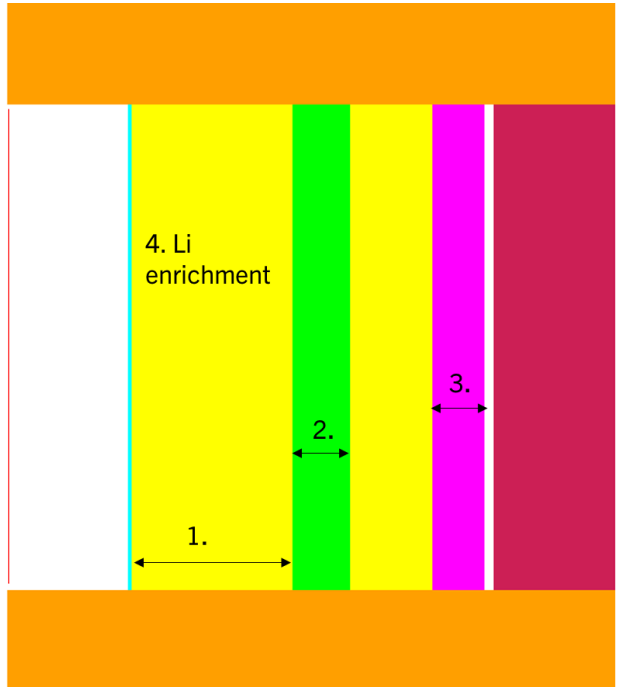
Application of DigiLab ML Model (Uncertainty Engine)



Trained model

Li1_th
BeTi_th
Shield_th
Li6_prop
…

MCBEND®

Blanket (FISPACT)

Incoming Inventory:
Trit
He
Li6
Li7
…

Purifier

Pipework

Outgoing Inventory:
Trit, He, Li6, Li7, ..

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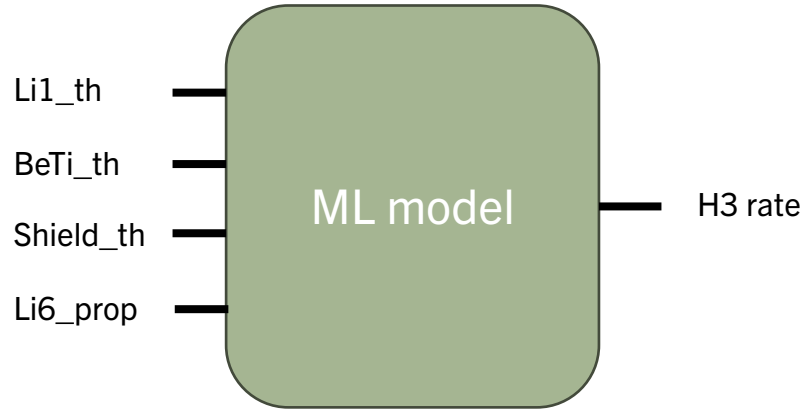
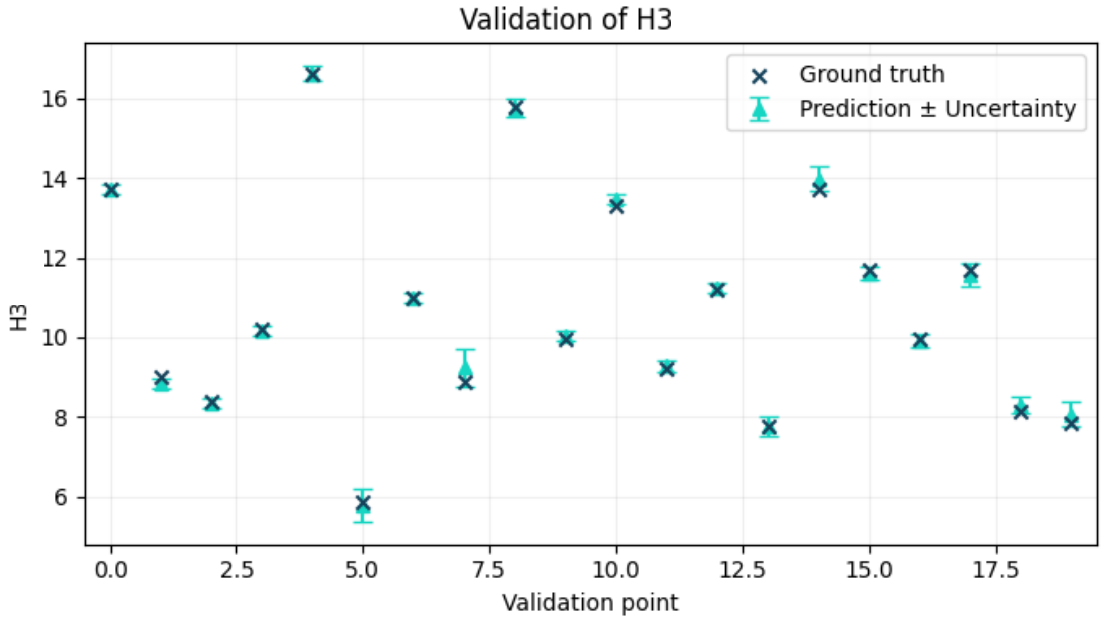
Model training

- Latin-hypercube sampling (100 samples) from:
  - Li1_th, BeTi_th, Shield_th, Li6_prop
- Training: 80 samples
- Validation: 20 samples
- R^2 - value: 0.997: model very well trained





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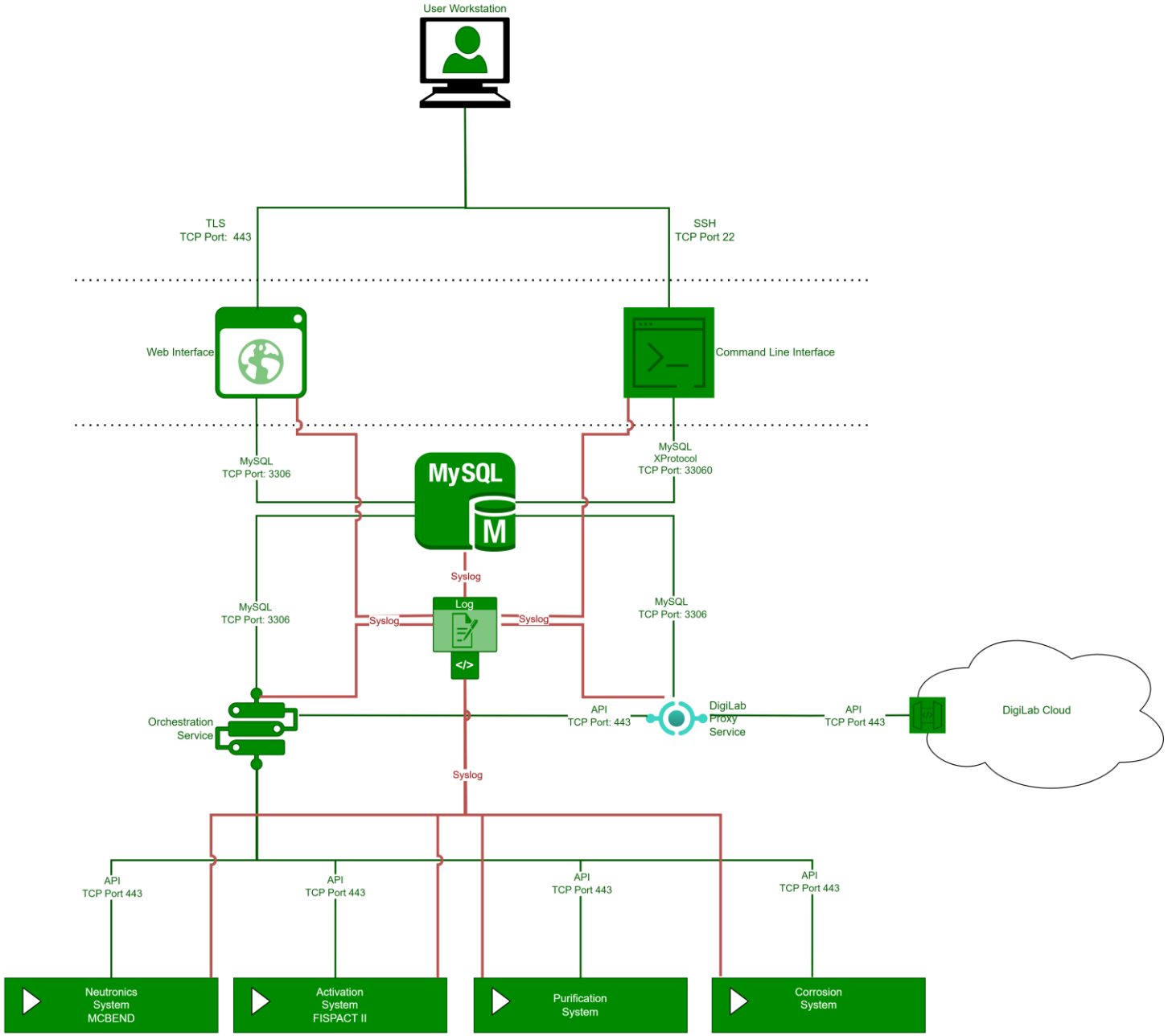
Software Infrastructure

- Secure software infrastructure developed
- Modular approach
- Integration of simulation engine
- GUI
- Workflow management
- Database for all simulation data
- Link to DigiLab services



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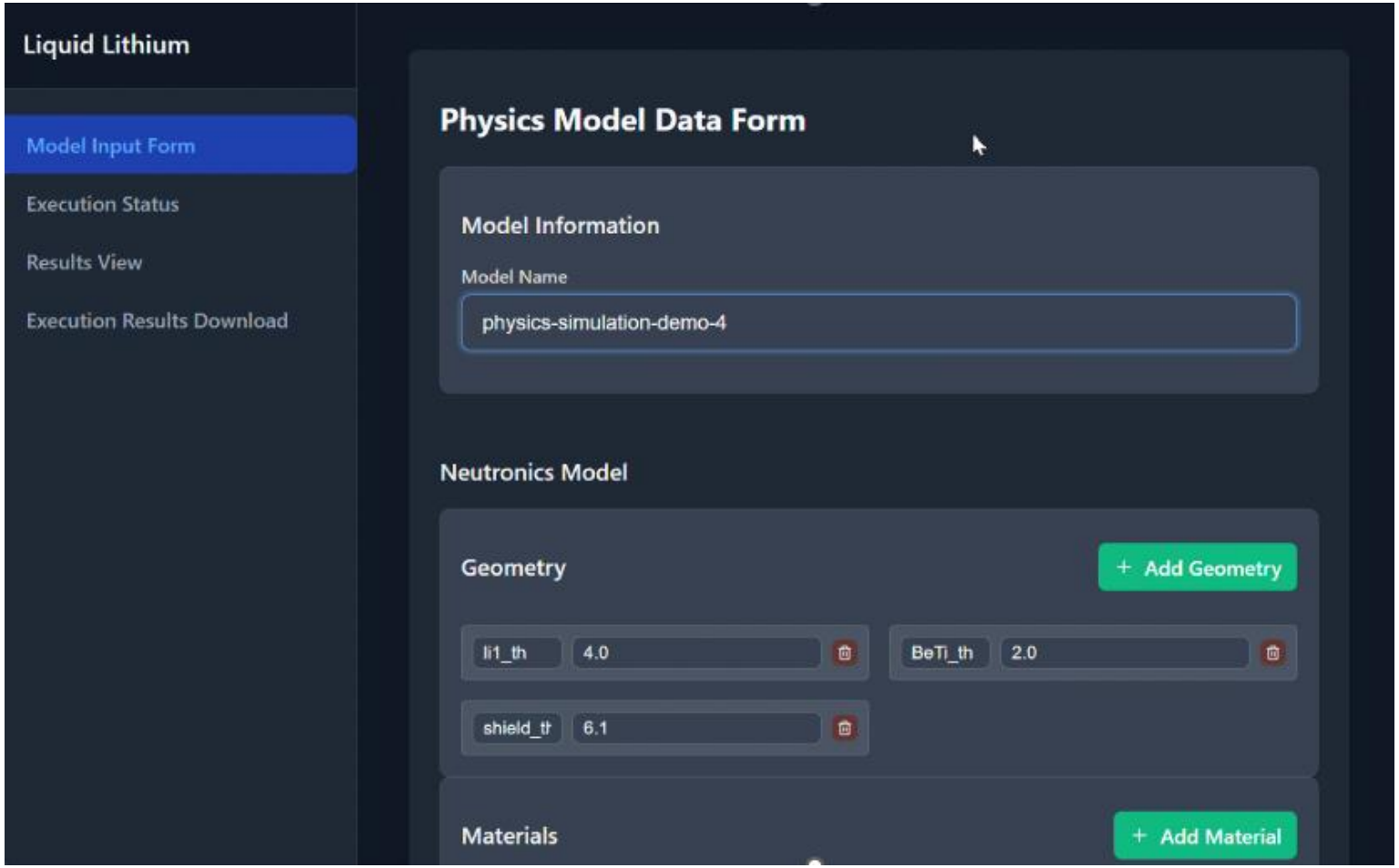
GUI (1)



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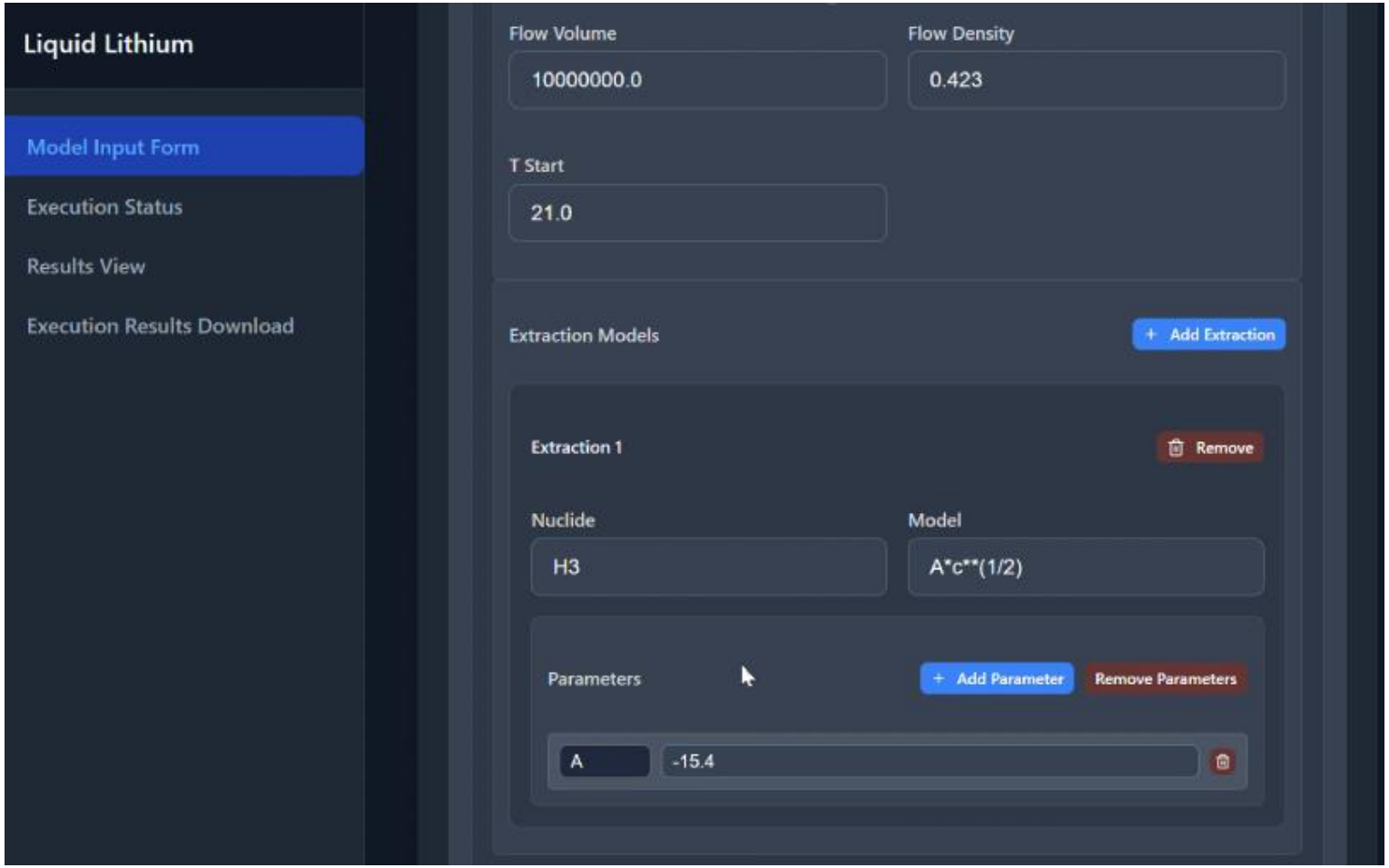
GUI (2)



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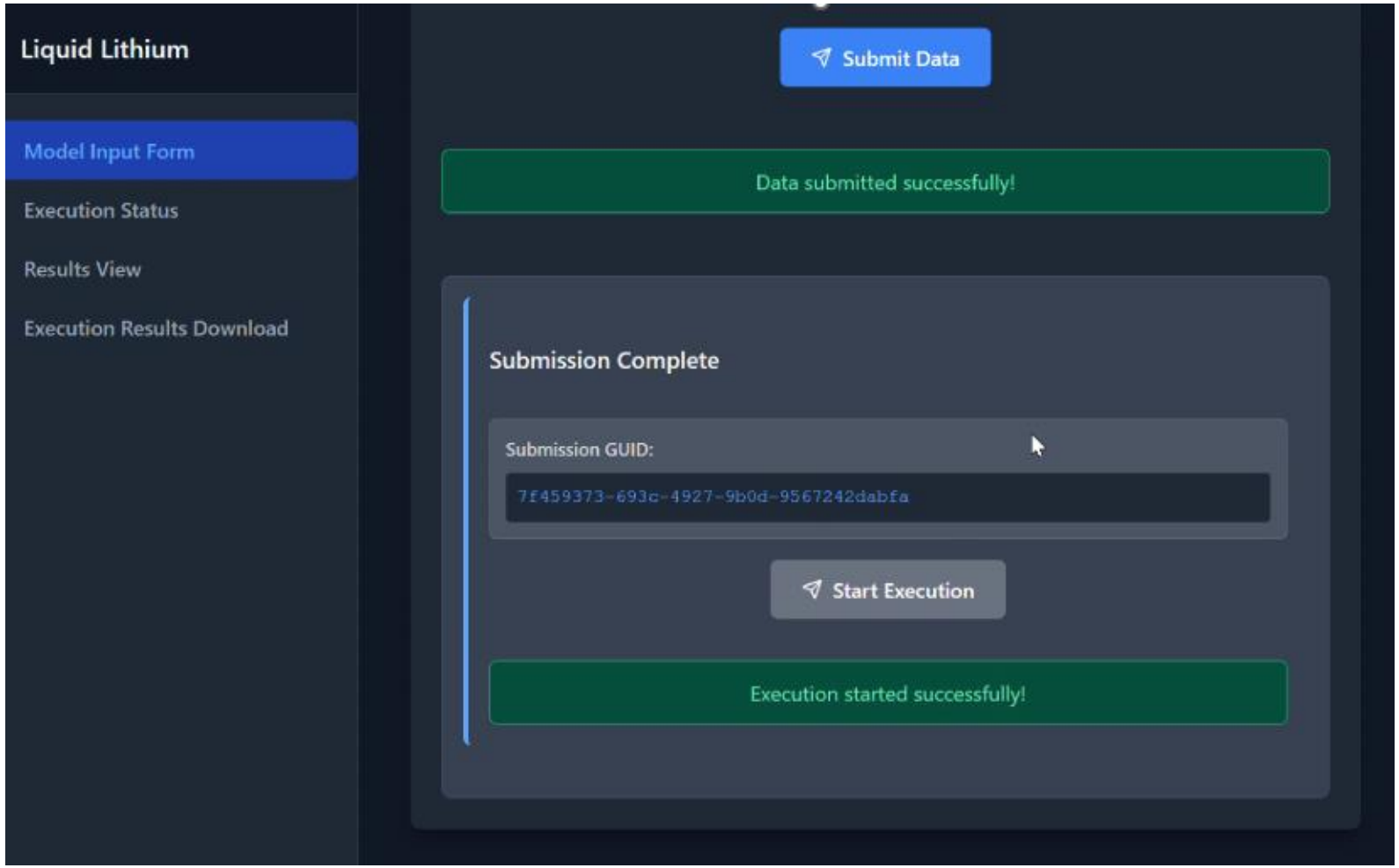
GUI (3)



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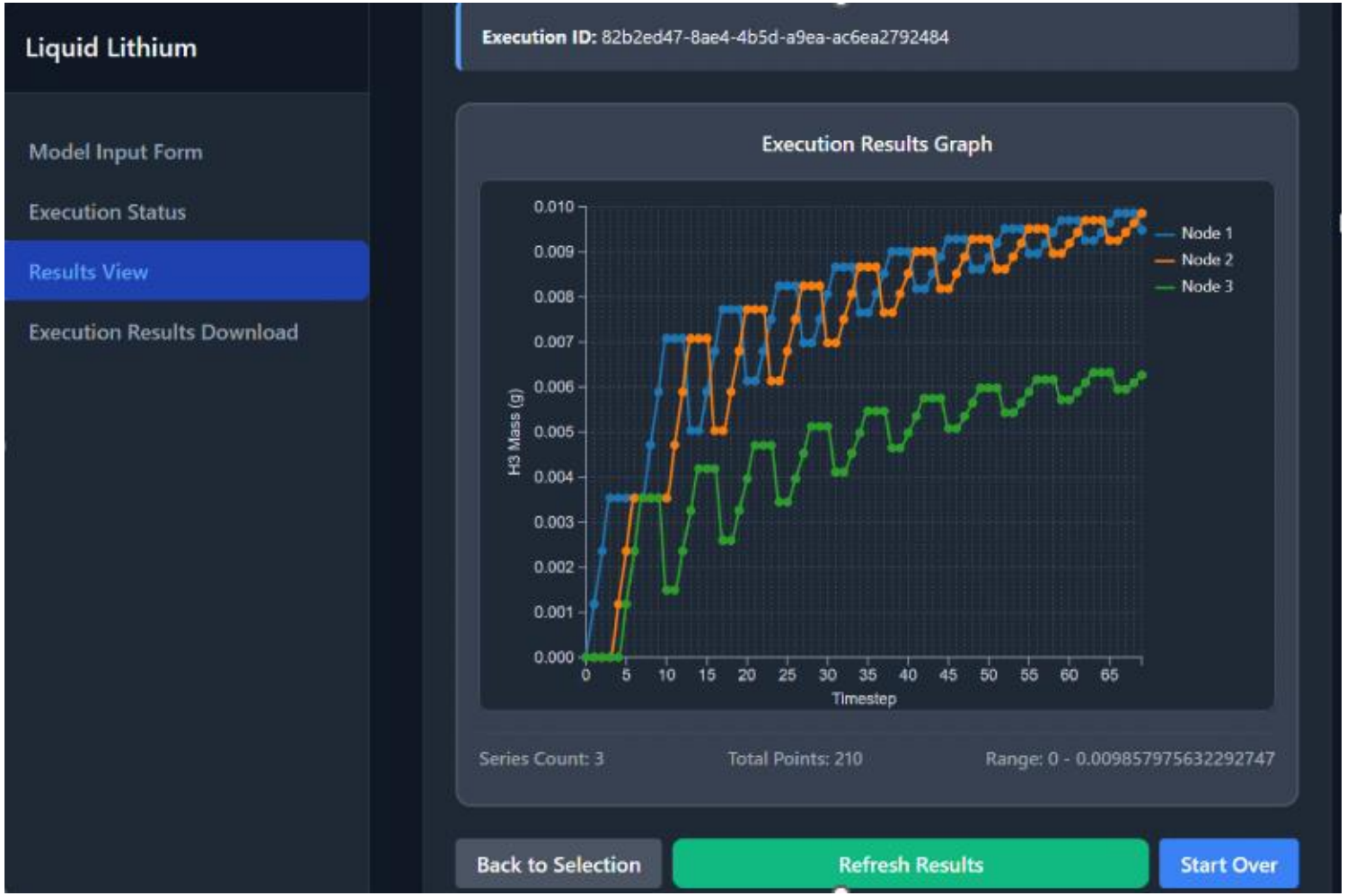
GUI (4)



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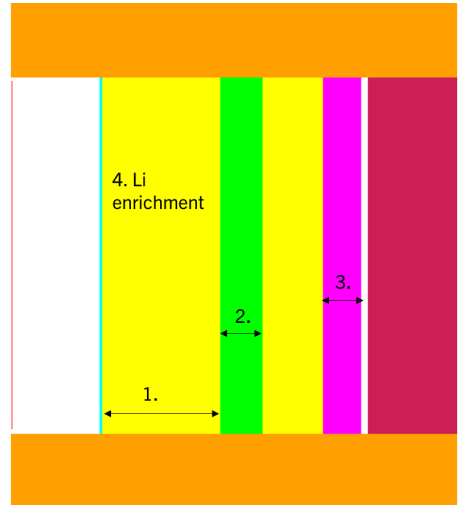
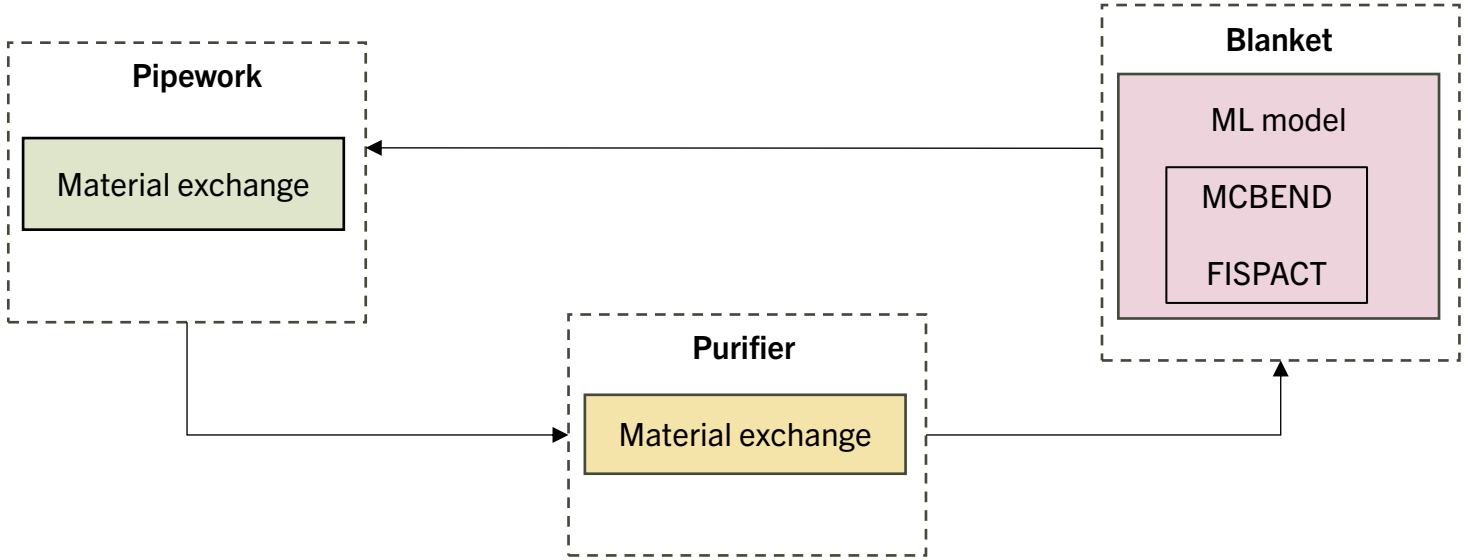
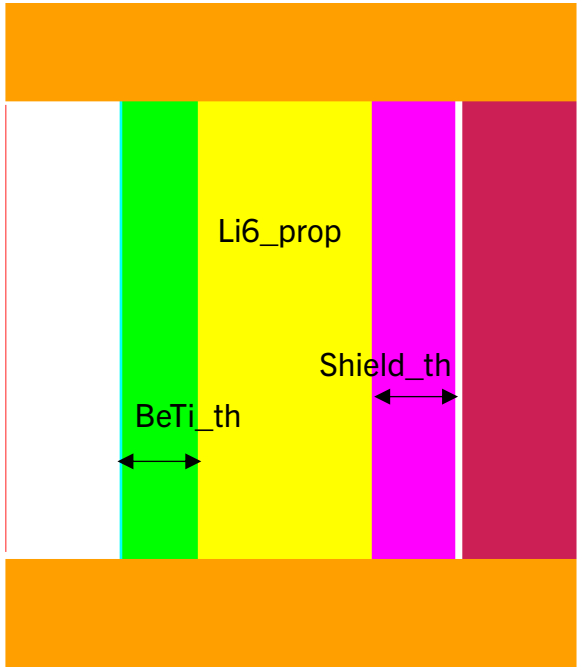
Demonstration application

- ML model successfully trained and accessible as simulation module
- Consider sub-group of blanket designs (only one Li region)
- Optimise blanket design: **maximum shield thickness for a target tritium yield**
- Each blanket design requires neutronics evaluation and multiple timesteps
  - No ML model: Many potentially very long (hours) Monte-Carlo (MCBEND) neutronics calculations
  - With ML model (seconds): **significant speed up**





Li6_prop
BeTi_th
Shield_th



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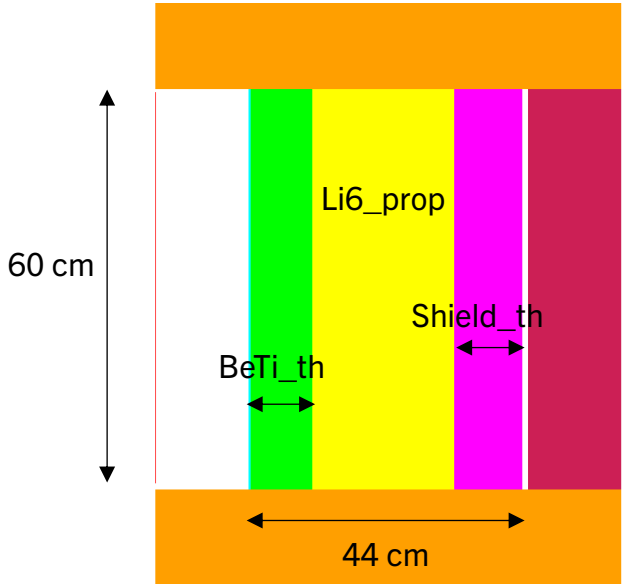
Demonstration application cont'd

- 300 samples of
  - Li6_prop
  - BeTi_th
  - Shield_th



- Li volumes
  - blanket (avr) : pipework : purifier = 30 : 10 : 3
- Tritium extraction / leakage rates:
  - Tritium leakage from blanket and pipework modelled
  - Extraction from Purifier
  - Rates: ~ Vol x $\sqrt{H3\ conc}$

- For each geometry: equilibrium tritium extraction rate determined

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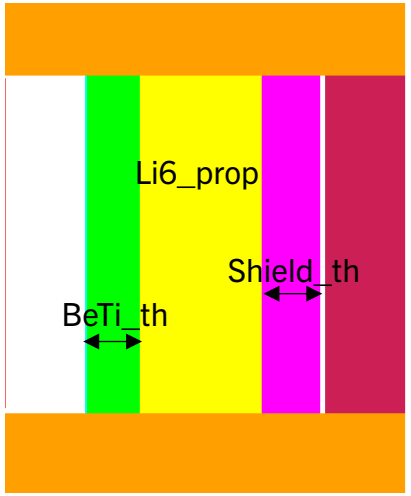
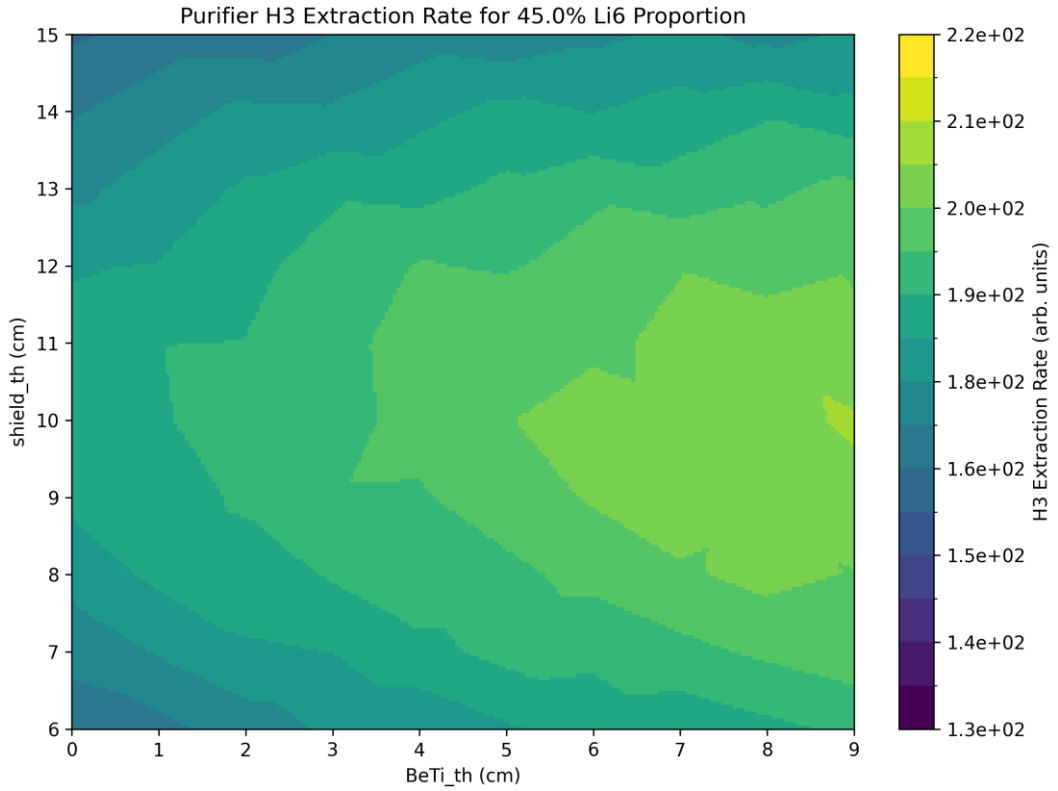
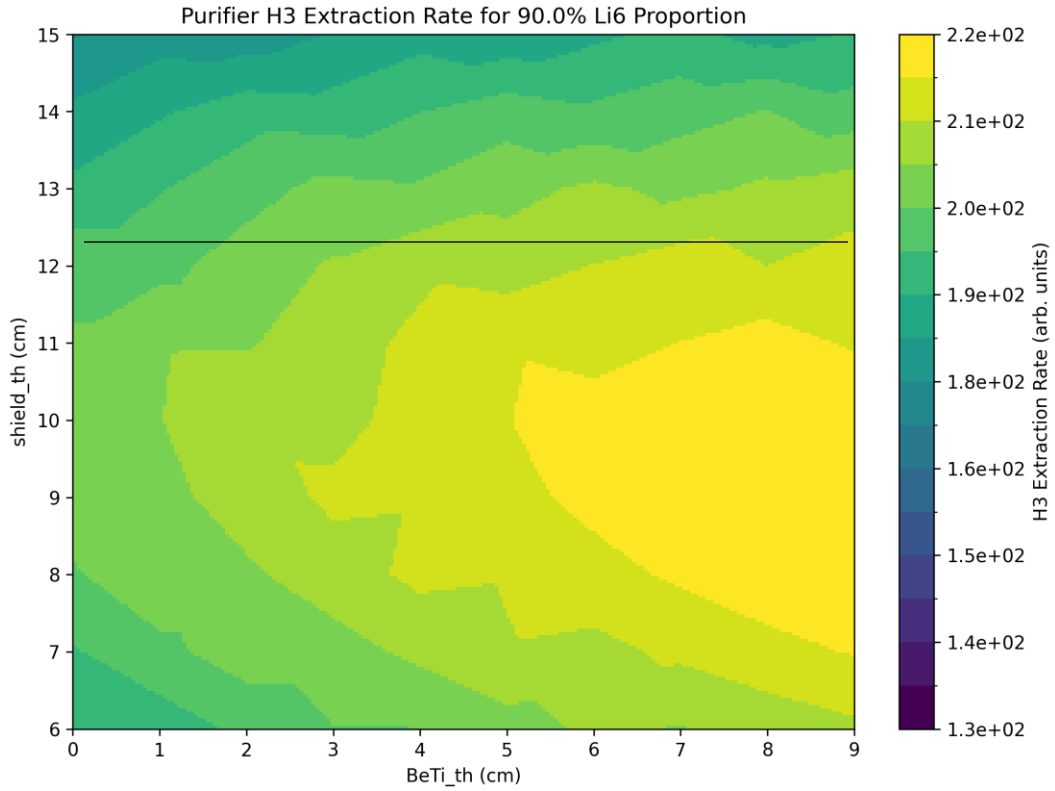
Demonstration application – Results

- ‘What is the maximum shield thickness at given Li6 prop and target H3?’
  - E.g.: H3 > 2.1E2 @ 90% Li6: shield_th < 12.2 cm
- Or: ‘What min Li6 prop is required given a target shield_th and H3 ?’







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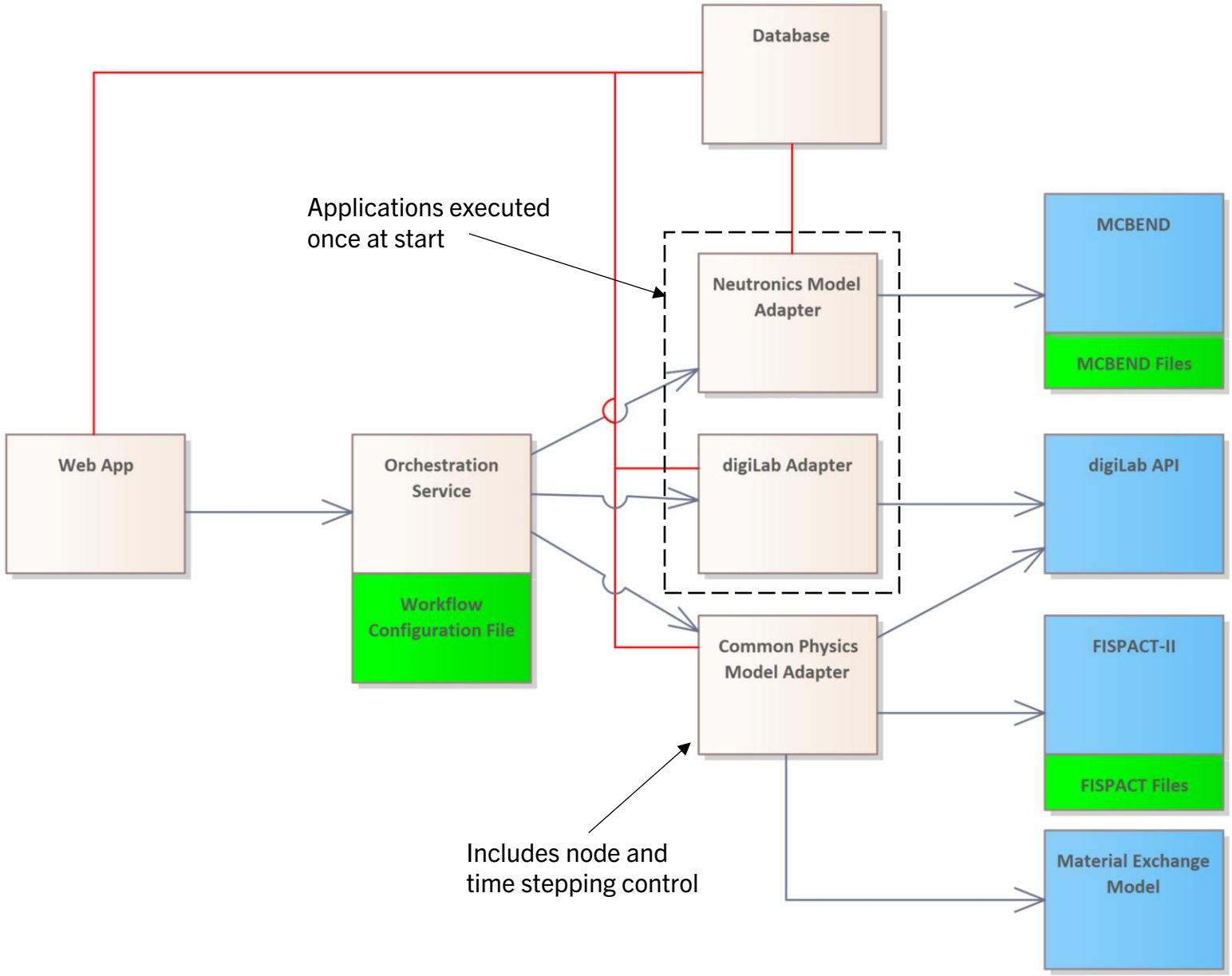
MOOSE integration - Current infrastructure

- Prototype implementation focussed on selected physics
- Workflows configurable with different sets of simulation apps

- MOOSE = powerful framework to integrate various physics

- Integration of MOOSE apps would allow
  - More detailed simulations
  - Benefitting from integration standard
  - Integrating existing tools more easily



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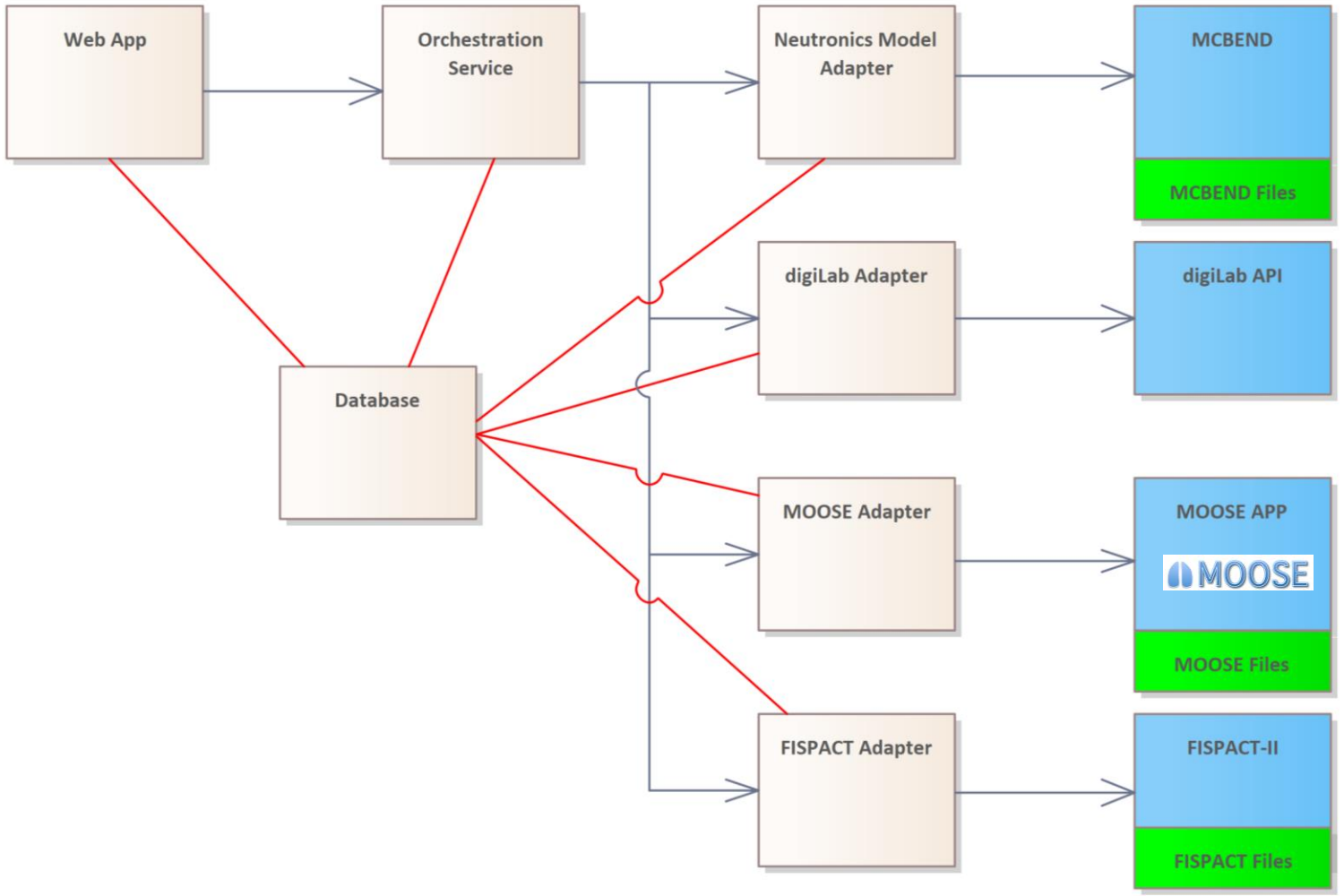
MOOSE integration - Planned extension

- Streamlined orchestration
- Workflow definition in database
- Integration of generic MOOSE application
- Flexible generation and use of surrogate models



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Conclusion

- LIBRTI programme: Develop facility to accelerate technology development for tritium breeding
- Digital Shadow / Twin of liquid lithium breeding solutions to support their development (planning / design / optimised data collection / validation / decommissioning)

- Simulation engine implemented using MCBEND® and FISPACT (example codes)
- Implemented **secure & flexible software infrastructure** supporting the simulation engine
- ML models (DigiLab) for neutronics/activation enable **significant speed up of design optimisation process**
- First steps taken towards **data-driven corrosion model**

- **Developed simulation platform not restricted to liquid lithium breeder designs – adoptable to other systems**
- Planned: integration of generic MOOSE applications to integrate more (detailed) physics / existing simulations

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Acknowledgments

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- The LIBRTI program for supporting this work under the ‘Small Scale Experiments for Tritium Breeding’ scheme
- DigiLab for their comprehensive support
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  - Zinnia Parker
  - Tom Cooper
  - Sarah Harrison
  - Ed Norfield
  - Noah Callow
  - Liban Ahmed
  - Emma Wilkinson

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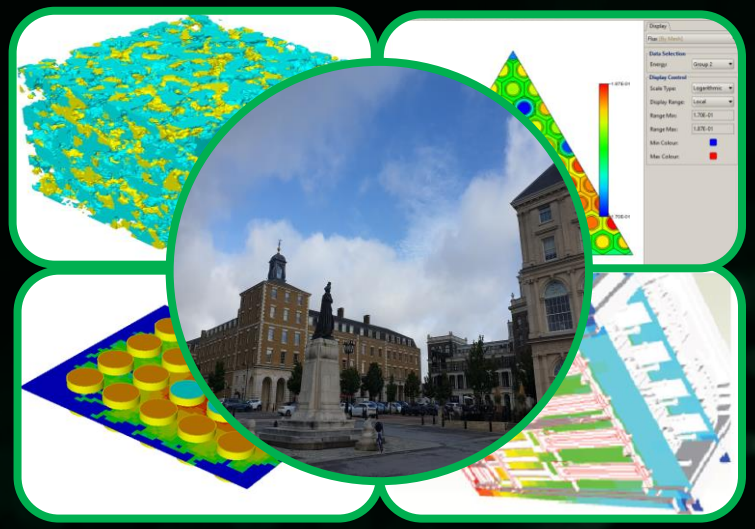

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