Plasma Science & Fusion Center

FESTIM
FINITE ELEMENT SIMULATION OF TRITIUM IN MATERIALS

Multi-physics tritium transport modelling of the ARC breeding blanket with FESTIM

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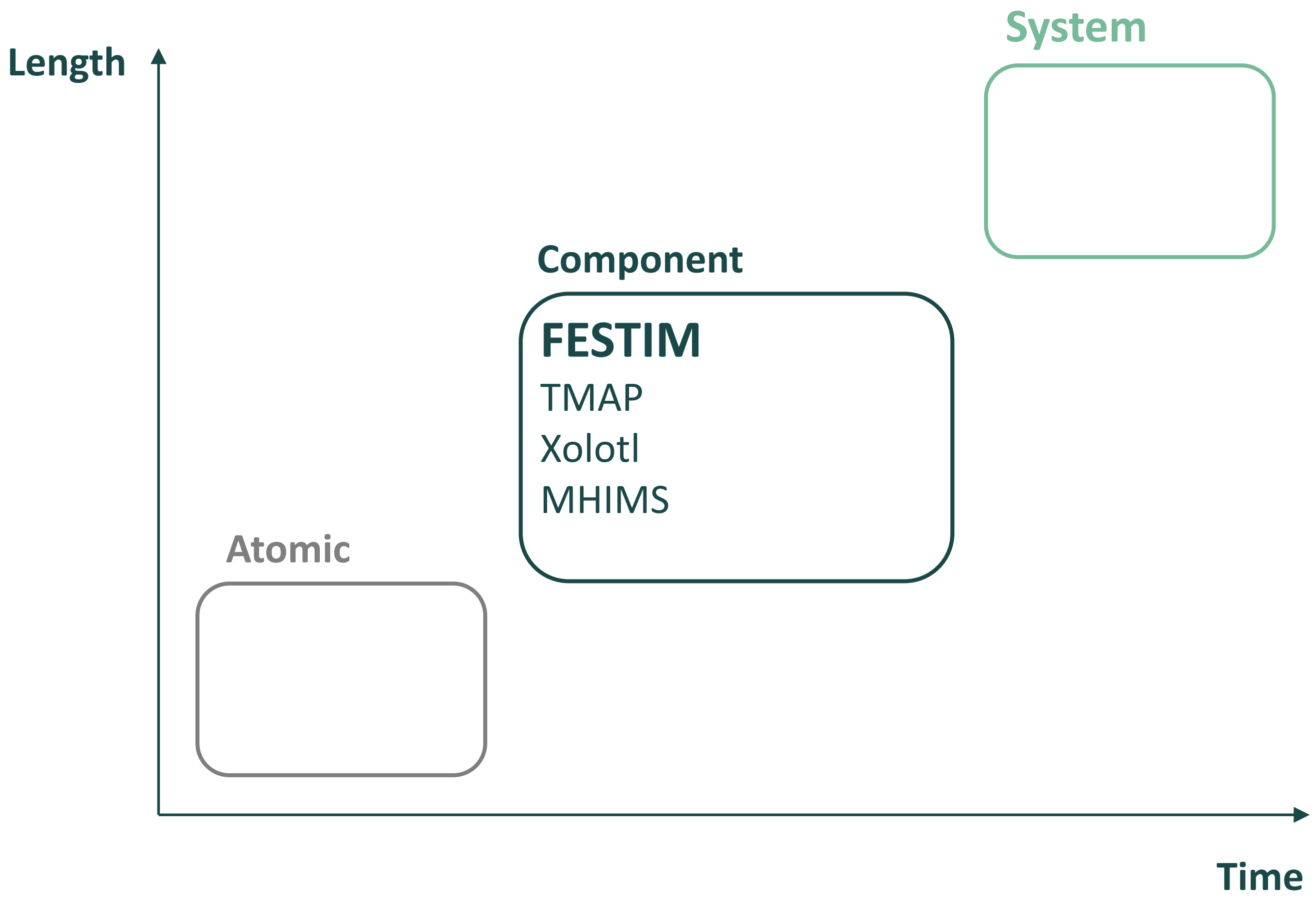
IAEA Workshop on Digital Engineering for Fusion Energy Research, Dec 9-12, 2025

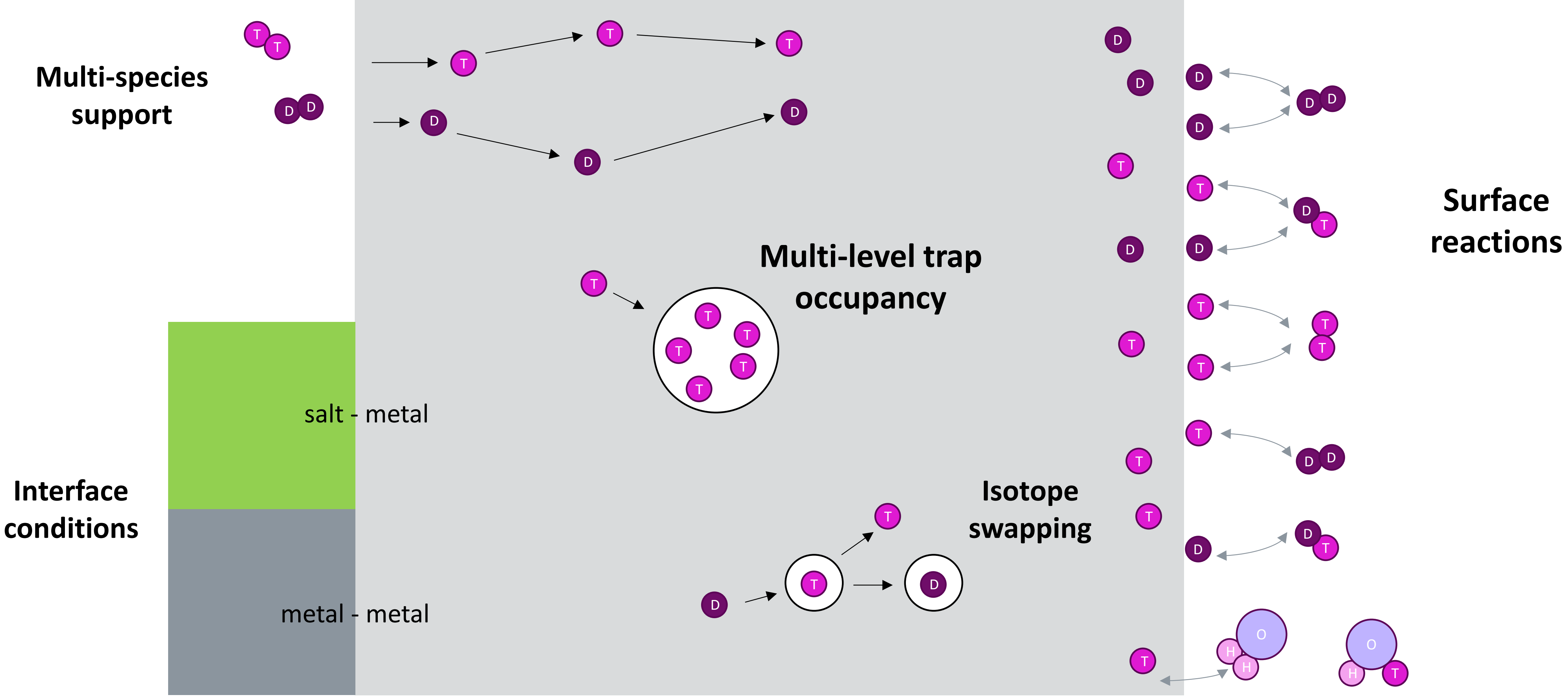
MIT | Cambridge, Massachusetts, USA

IAEA

Multiscale tritium transport modelling



Tritium transport capabilities in FESTIM



FESTIM

NUMFOCUS
OPEN CODE = BETTER SCIENCE

Performance

- ⚡ **FEniCSx** - JIT to fast C++ rapid assembly
- 🚀 **High-performance solvers** - PETSc back-end
- **Built for HPC** - Native MPI, runs on 1000's of cores
- 🧩 **Tuned control** - Custom meshes, solvers, finite elements
- 📦 **Fast I/O** - Parallel mesh loading, low memory footprint

Usability

- **User friendly -** Intuitive, Python API easy to use
- 📜 **Apache 2.0 license** - Suitable for academic *and* commercial
- ⚙️ **Easy install** - `conda install -c conda-forge festim`
- 💡 **Online tutorials** - Dozens of tutorials
- **Online documentation** - Auto-generated

Community

- **1,000+ forum views/month** - Public, searchable Q&A
- 🌎 **27+ institutions** - Adopted by universities, labs and industry
- **23+ contributors** - Open to new developers and users
- **Monthly dev meetings** - Community-driven roadmap
- **80+ Slack users** - Active developer and user support

Sustainability

- 🧱 **Built on FEniCSx** - Proven FEM backend, 1.5M+ downloads
- 🏋️ **5 team members at MIT**
- **On GitHub** - Transparent, version-controlled development
- 🤝 **NumFOCUS affiliation** - Backed by a sustainability non-profit
- 🔁 **CI/CD workflows** - Rigorous testing and streamlined releases

Modelling breeding blankets

- TBR calculations are important, but there's more!
- If tritium isn't extracted quickly, this will hinder the overall performance of the plant
- FESTIM helps us understand the tritium *dynamics*.

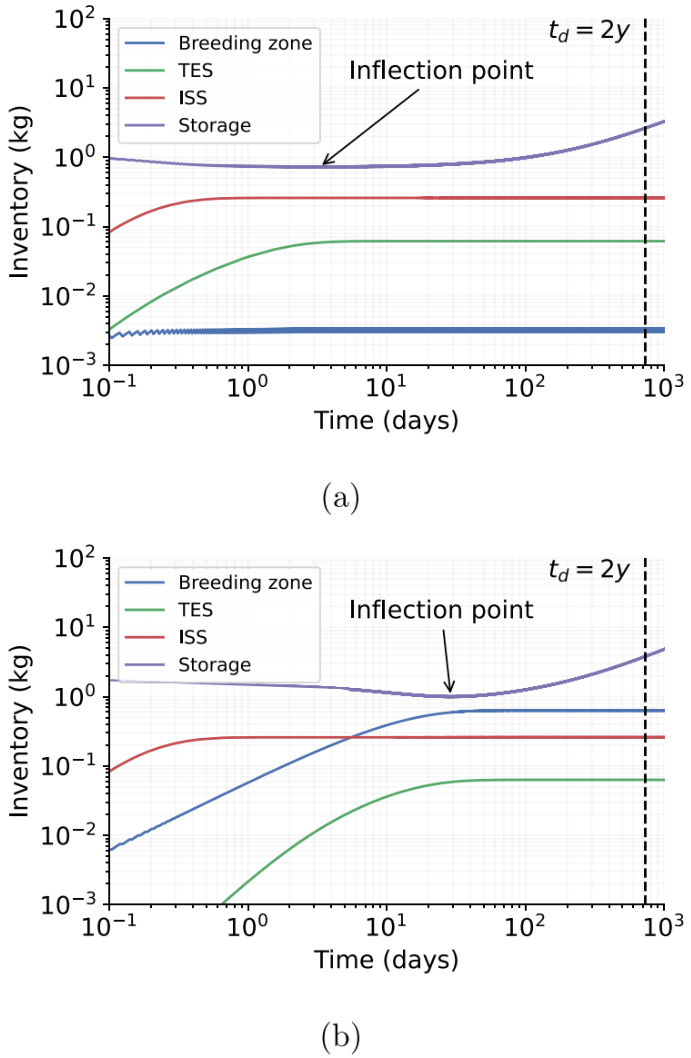
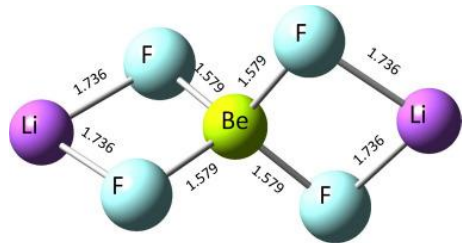


Figure 8. Evolution of relevant system inventories for (*a*) $\tau_{BZ} = 1.25$ h and (*b*) $\tau_{BZ} = 10$ d. The slower dynamics and the shift of the inflection time for $\tau_{BZ} = 10$ d is evident.

S. Meschini (2023) 10.1088/1741-4326/acf3fc

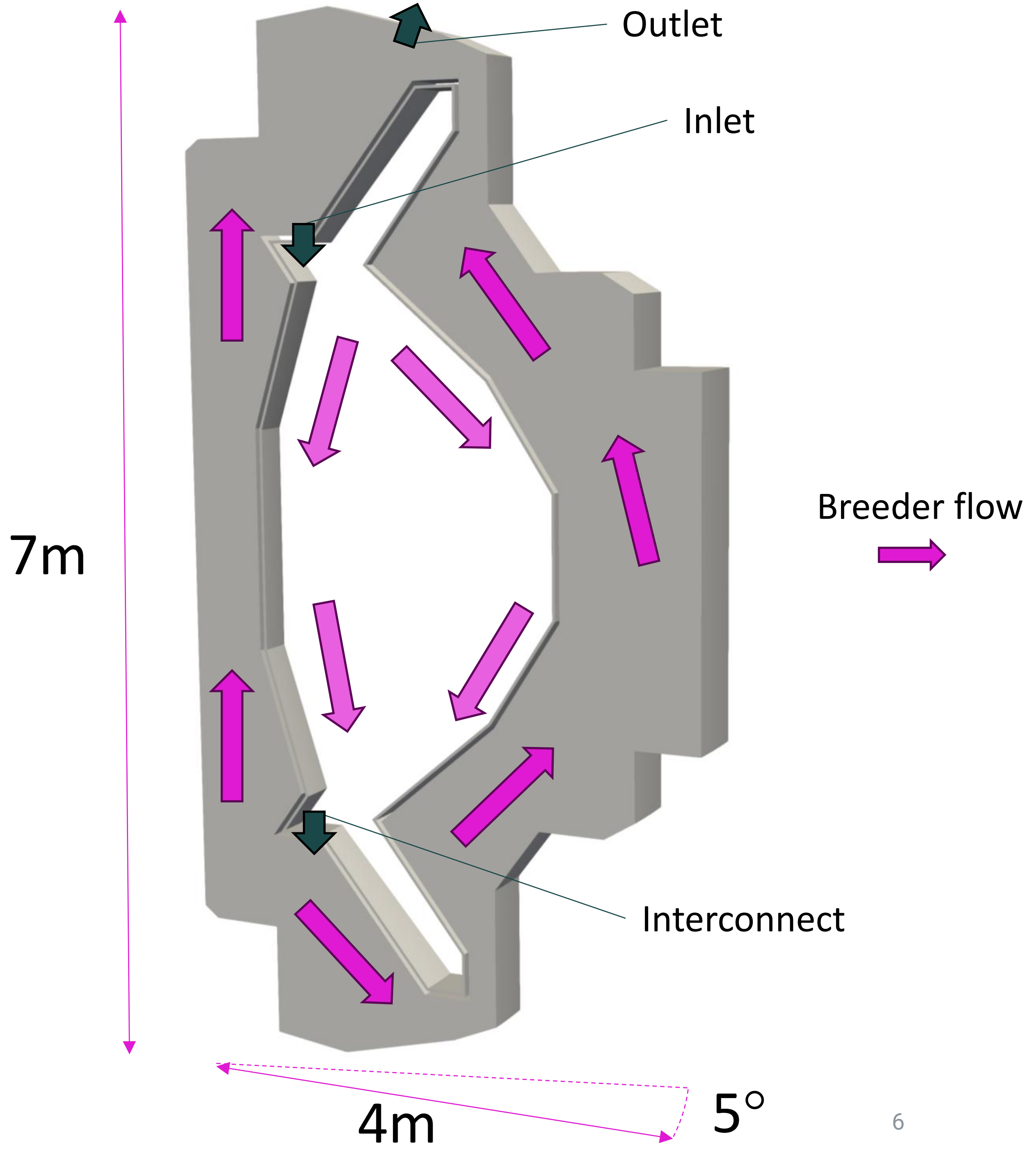
ARC model



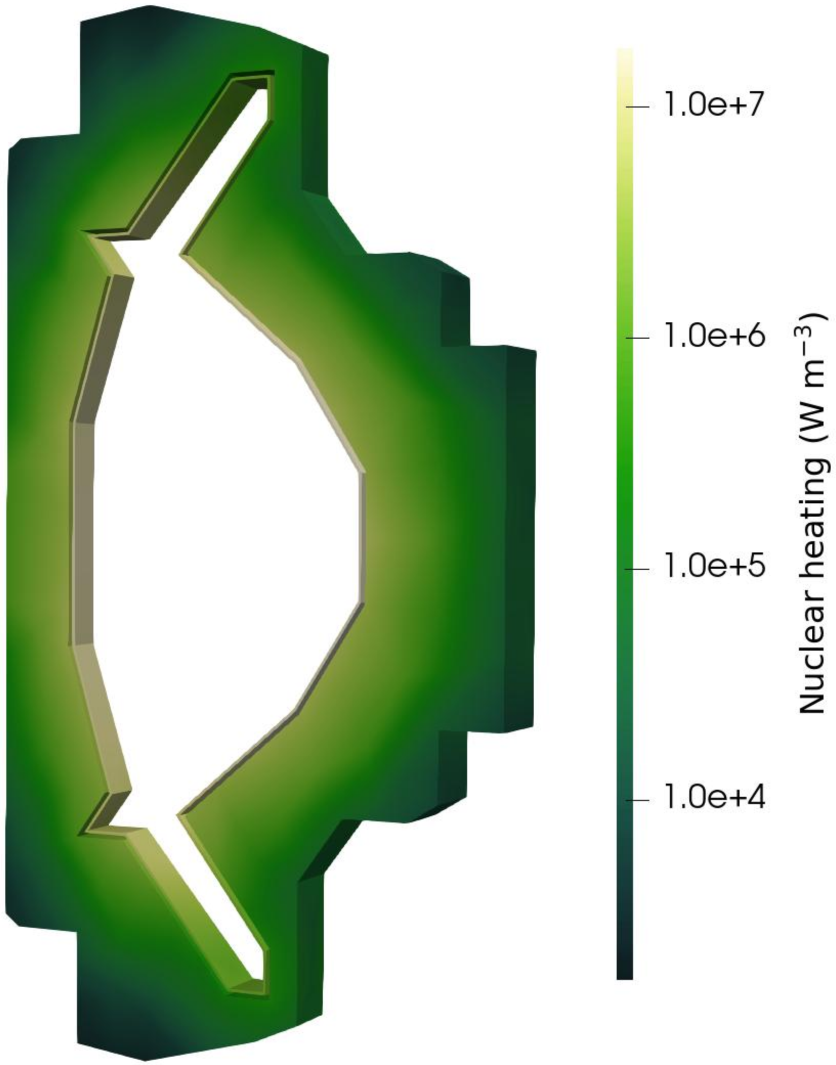
FLiBe breeder

525 MW

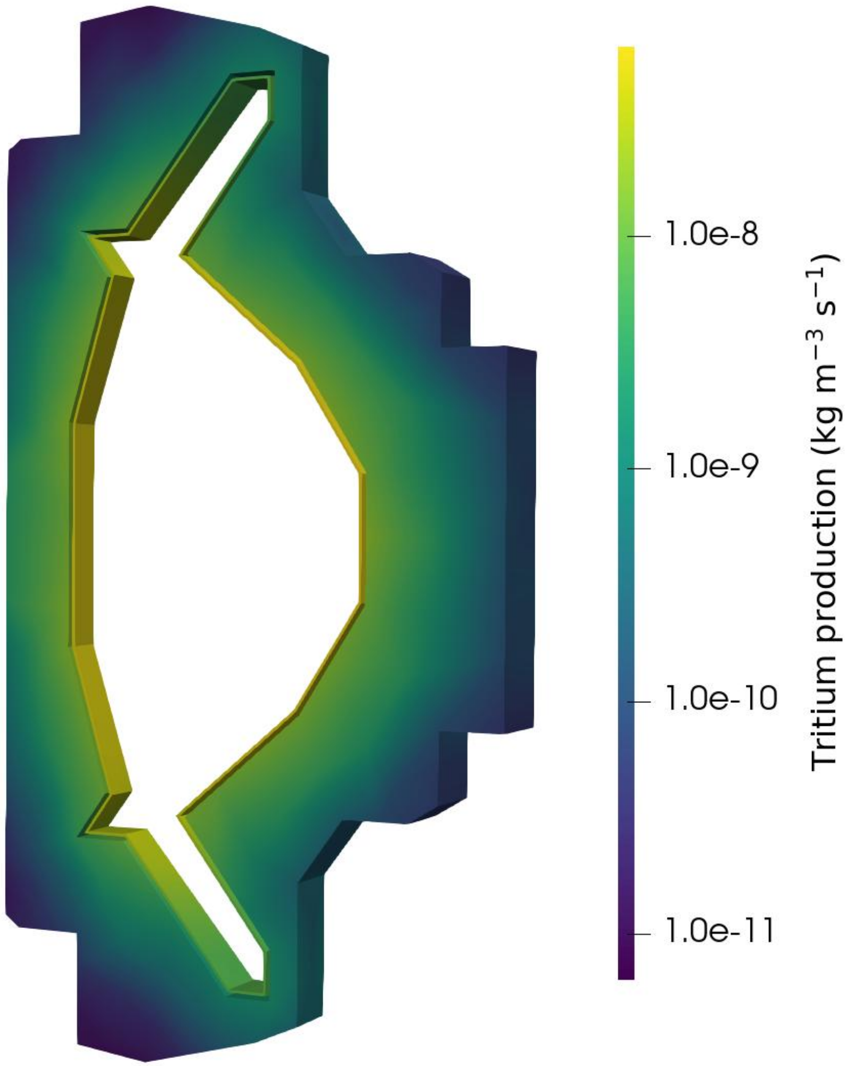
> **Note**
>
> No solid walls considered.



Neutronics



Nuclear heating

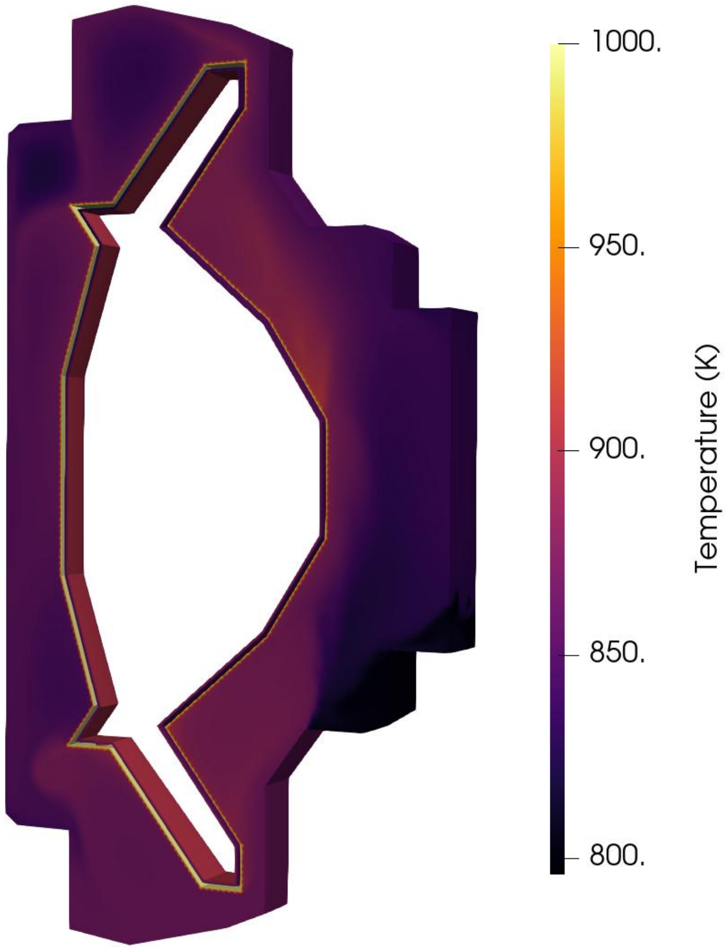


Tritium production

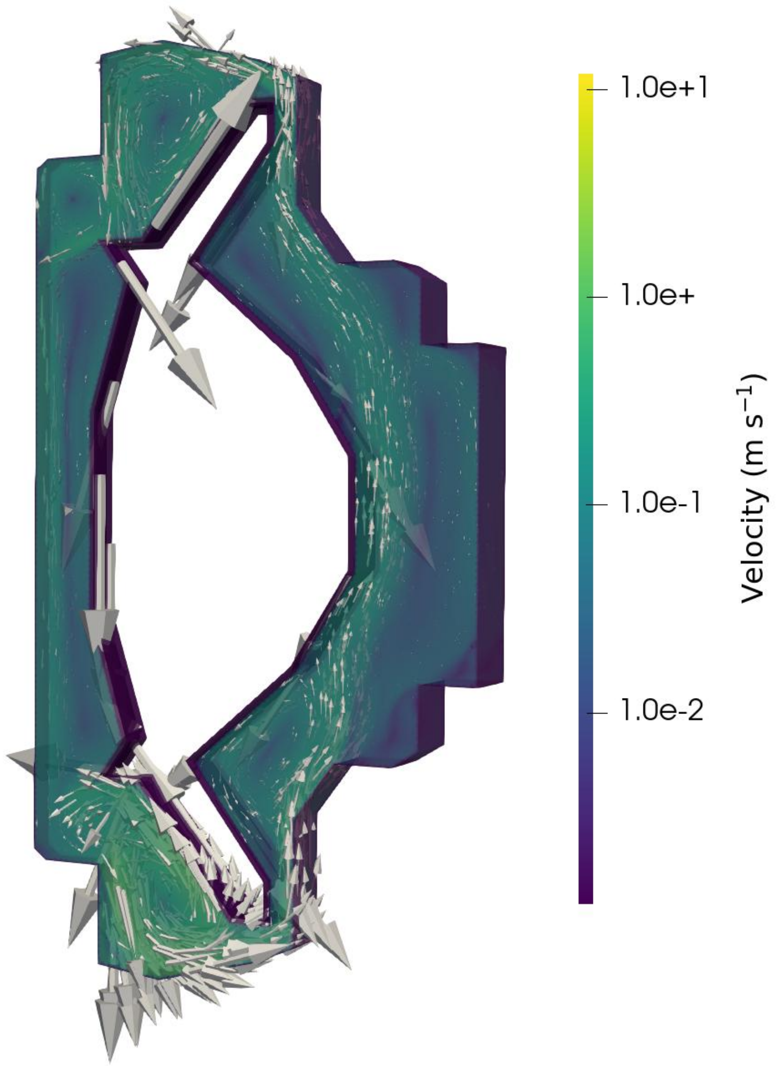
CFD

Oak Ridge National Laboratory

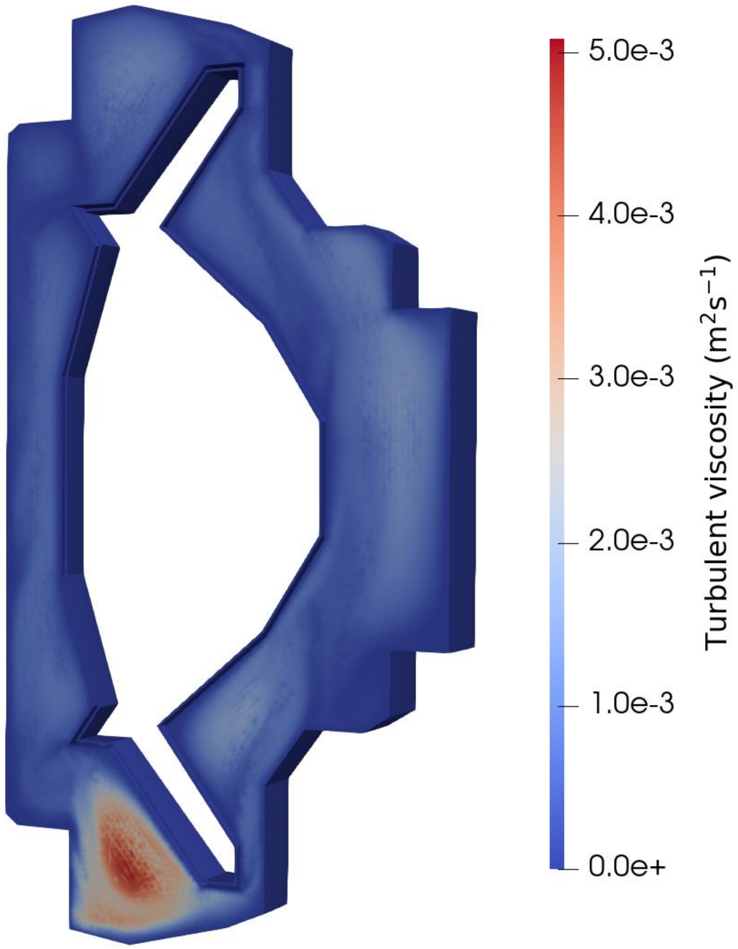
OpenFOAM



Temperature

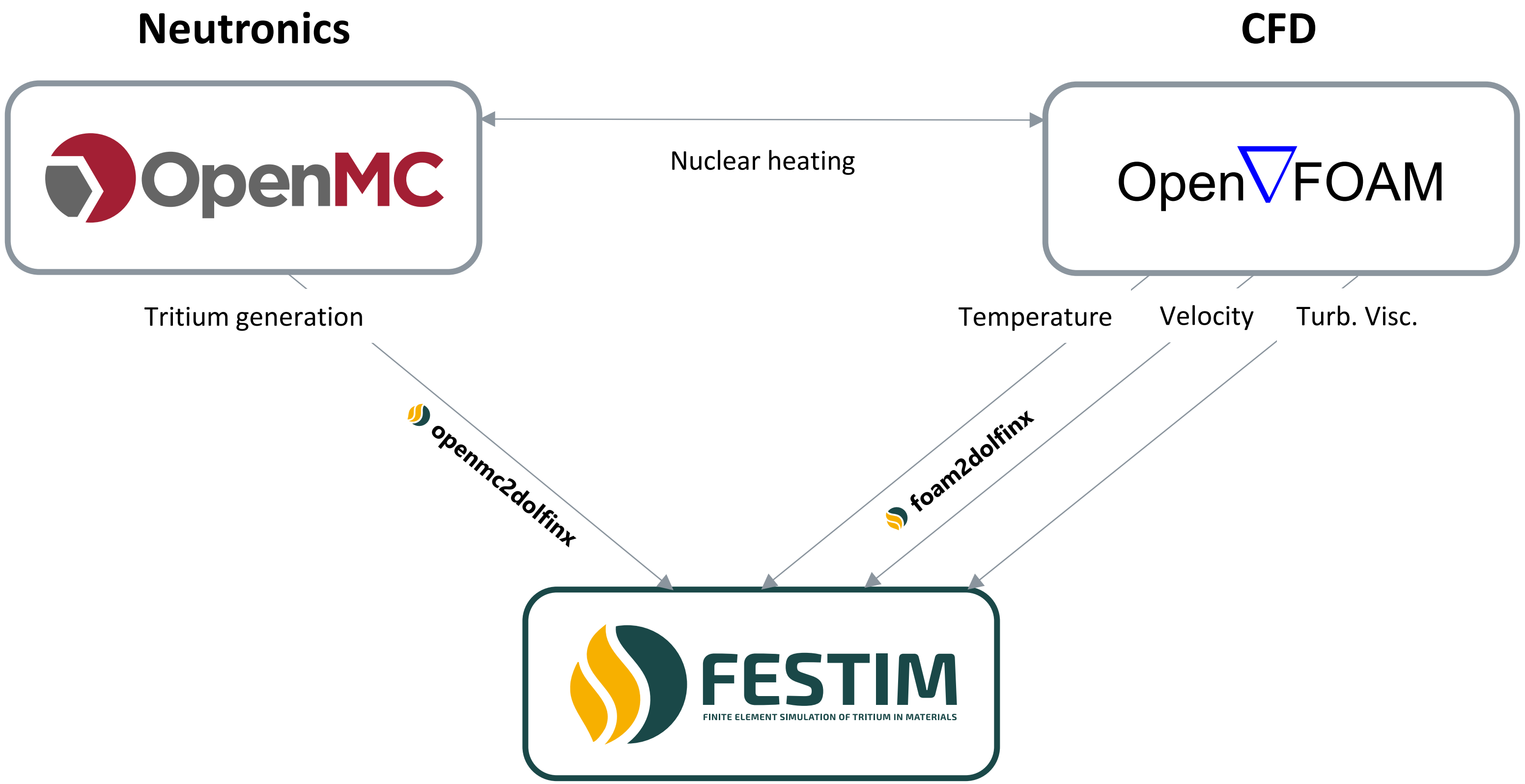


Velocity

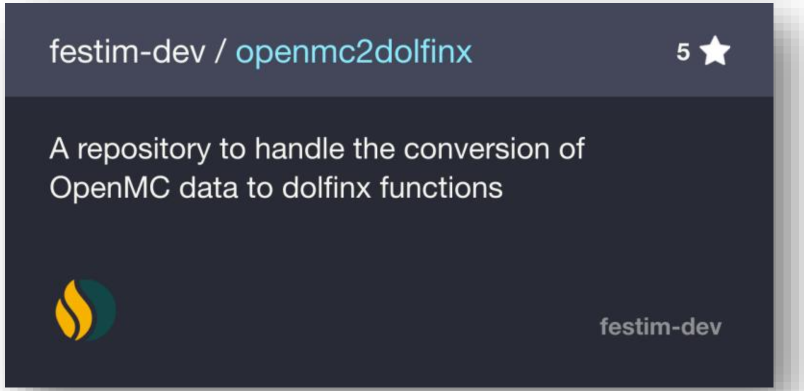


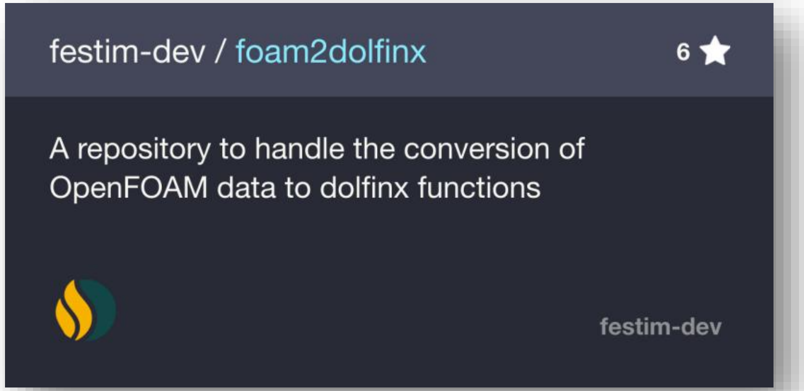
Turb. Visc.

Multi-physics coupling



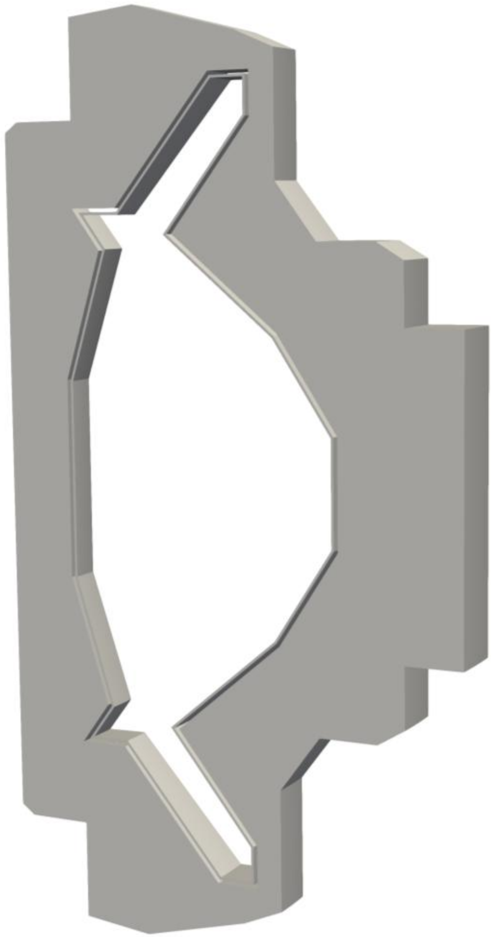
Openmc2dolfinx and foam2dolfinx





- Makes use of readers within **Pyvista**
- Maps data from a *.vtk* mesh to a FEniCSx mesh
- Works with both **structured** and **unstructured** meshes
- Interpolation can then be handled efficiently within FEniCSx

ARC breeding blanket: tritium model



$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) + S + u \nabla c$$

$$D(T) = \underbrace{D_0 \exp\left(\frac{-E_D}{k_B T}\right)}_{\text{Fickian}} + \underbrace{\frac{\nu_t}{\mathbf{Sc_t}}}_{\text{Turbulent}} + \underbrace{\boldsymbol{\delta} h||u||}_{\text{Stabilisation}}$$

Boundary conditions:

$c = 0 \quad \text{at inlet}$ (assumes perfect extraction system)

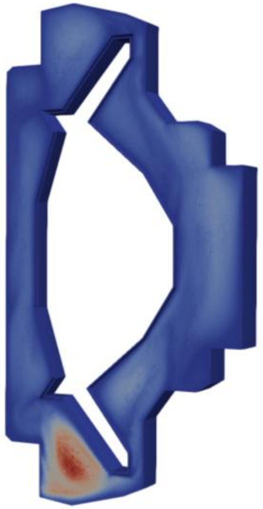
Material properties:

$D_0 = 6.75 \times 10^{-6}\ \mathrm{m^2 s^{-1}}$ $E_D = 0.615\ \mathrm{eV}$

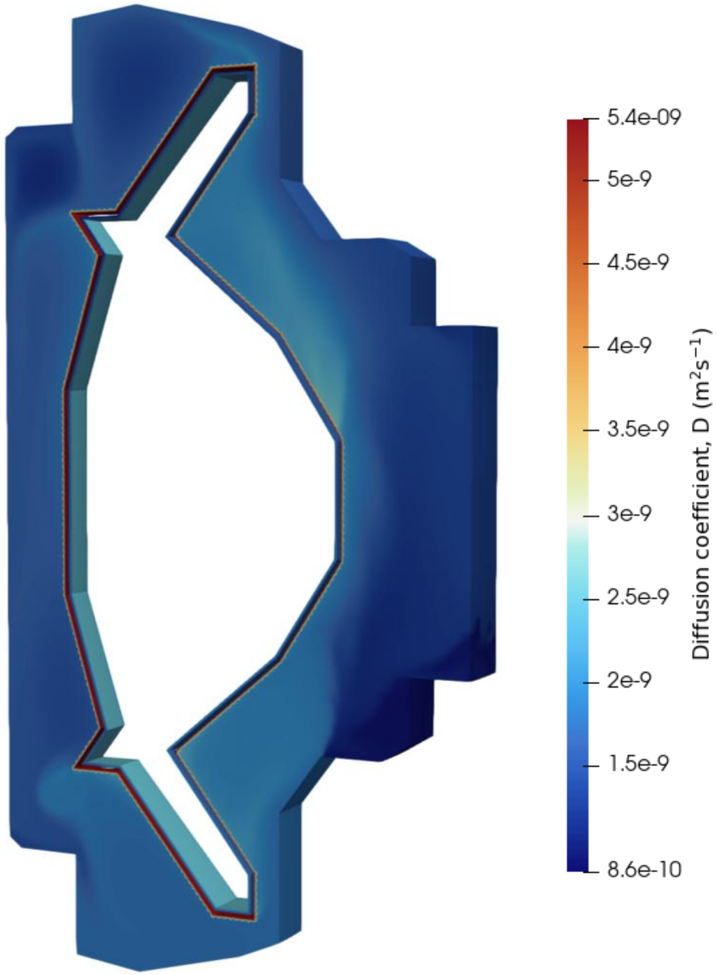
$\mathrm{Sc}_t = 0.5$

Fickian vs Turbulent diffusion

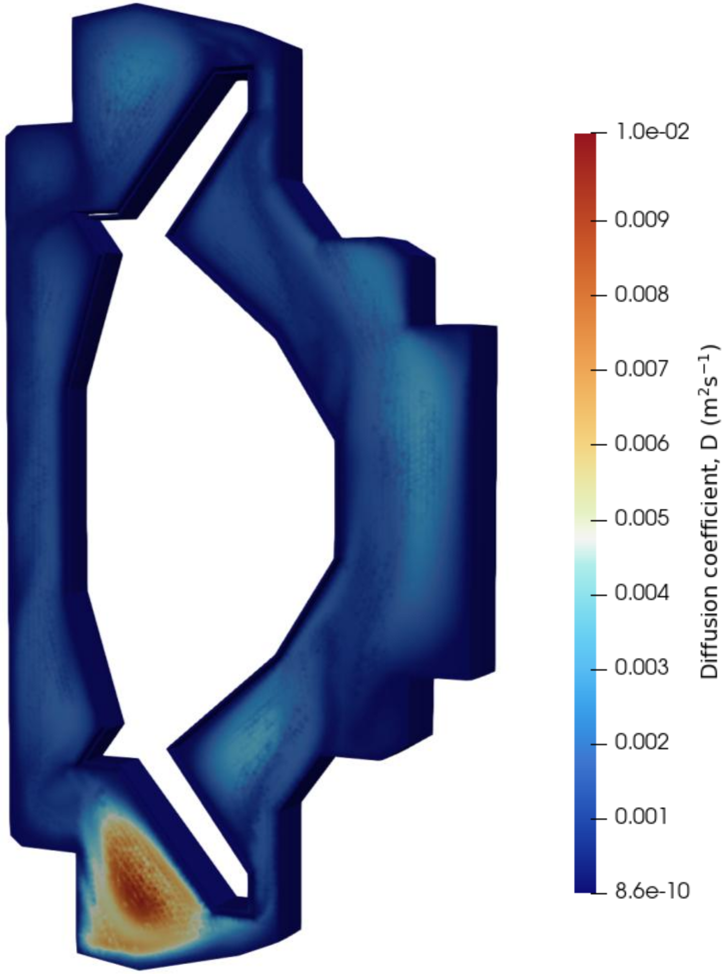
Temp.



Turb. Visc.



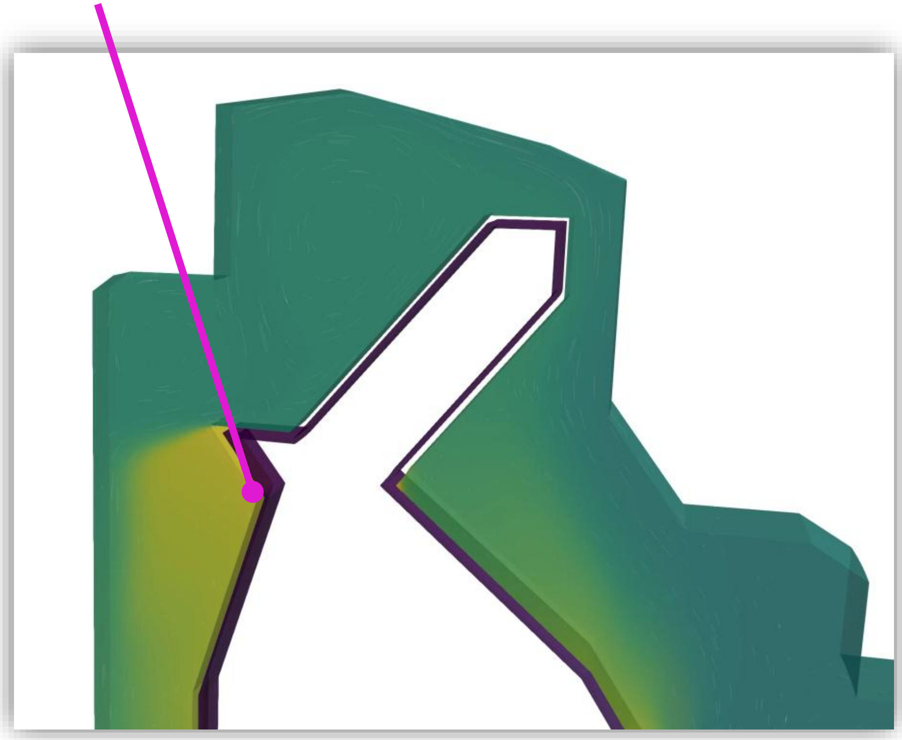
Fickian



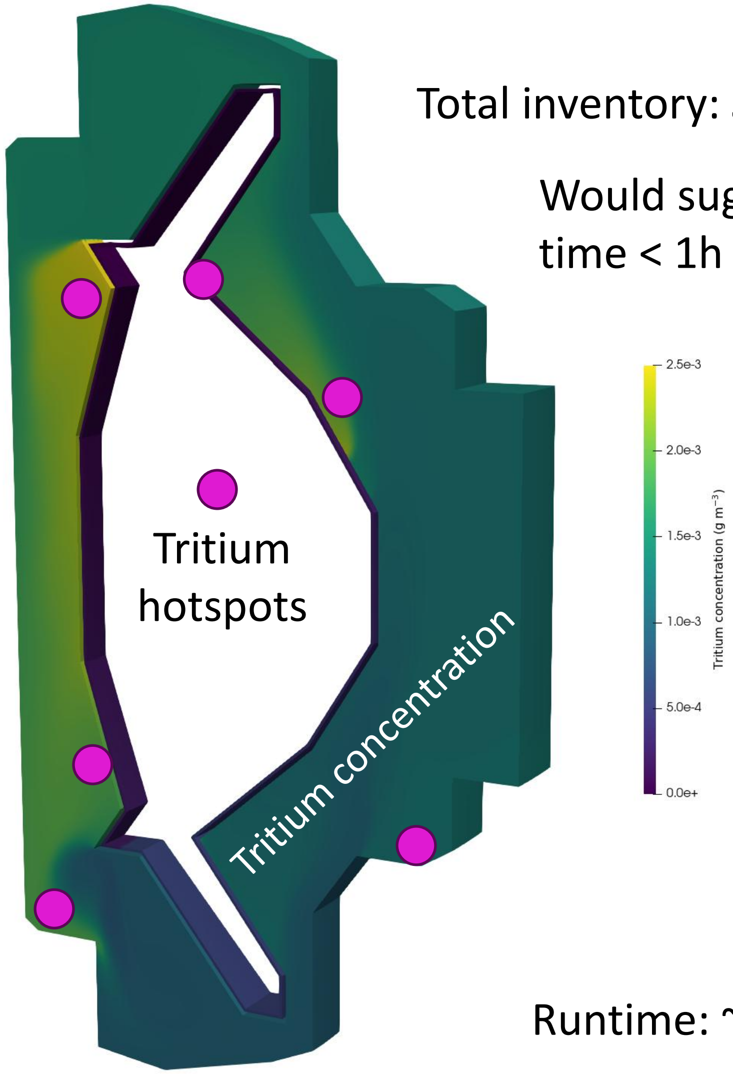
Fickian + Turbulent

FESTIM can help optimise blanket inventory

Max concentration:
1E-3 mol T/m3



Flow needs to be optimised to avoid stagnant salt

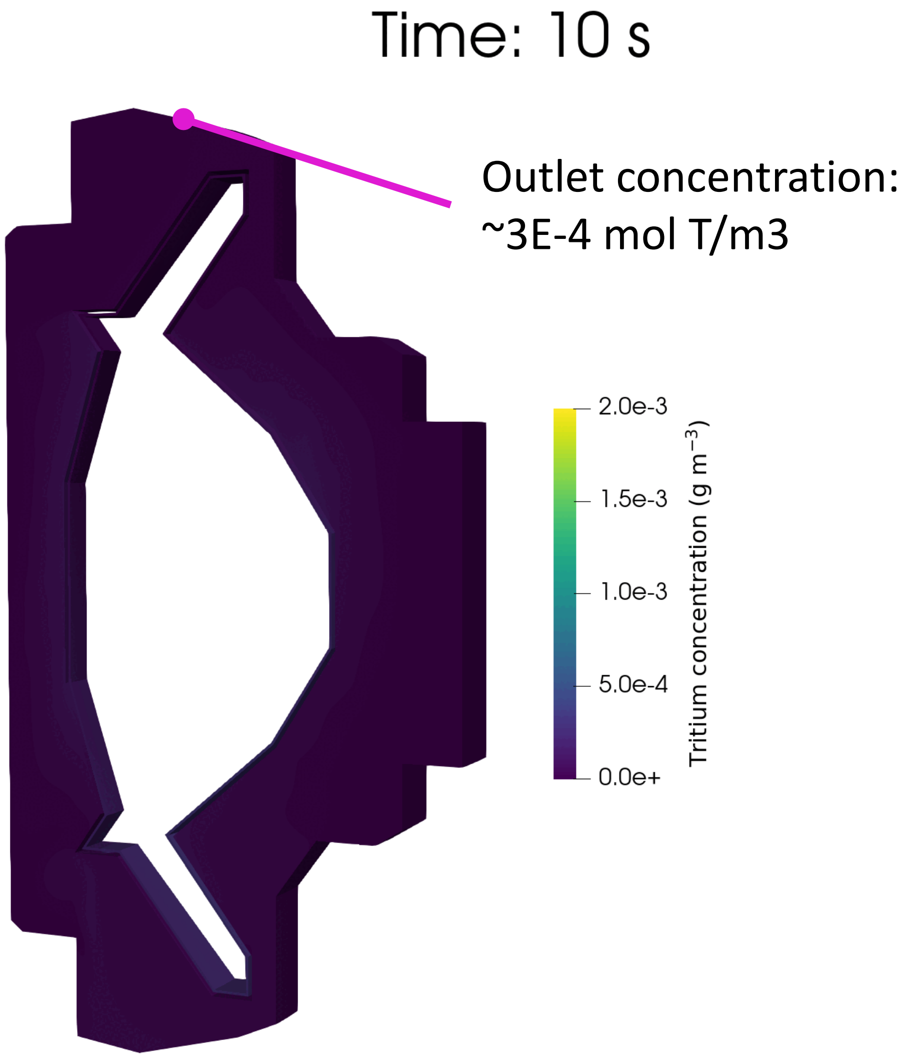


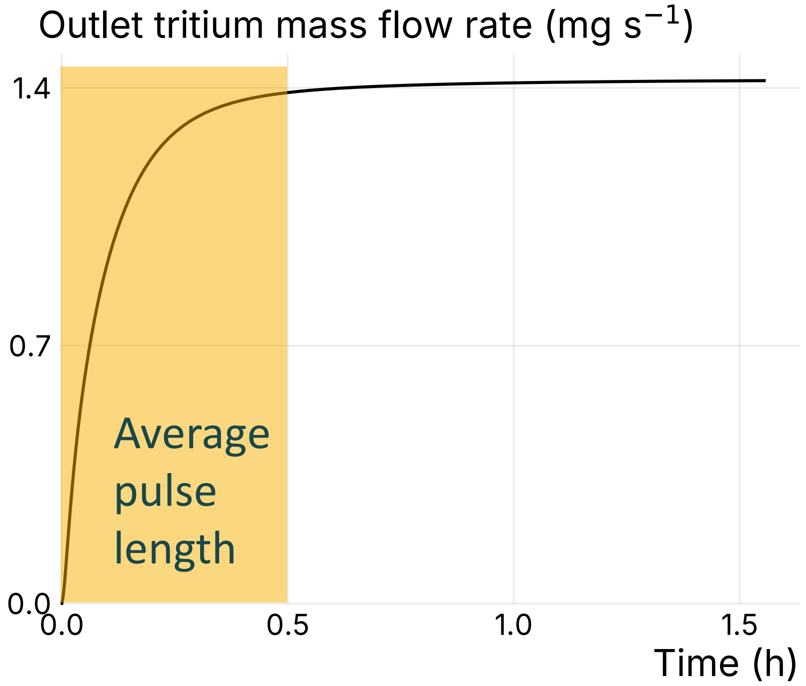
Total inventory: **390 mg T**

Would suggest residence time < 1h

Runtime: ~1 min (1 CPU)

We can also analyse the transient dynamics





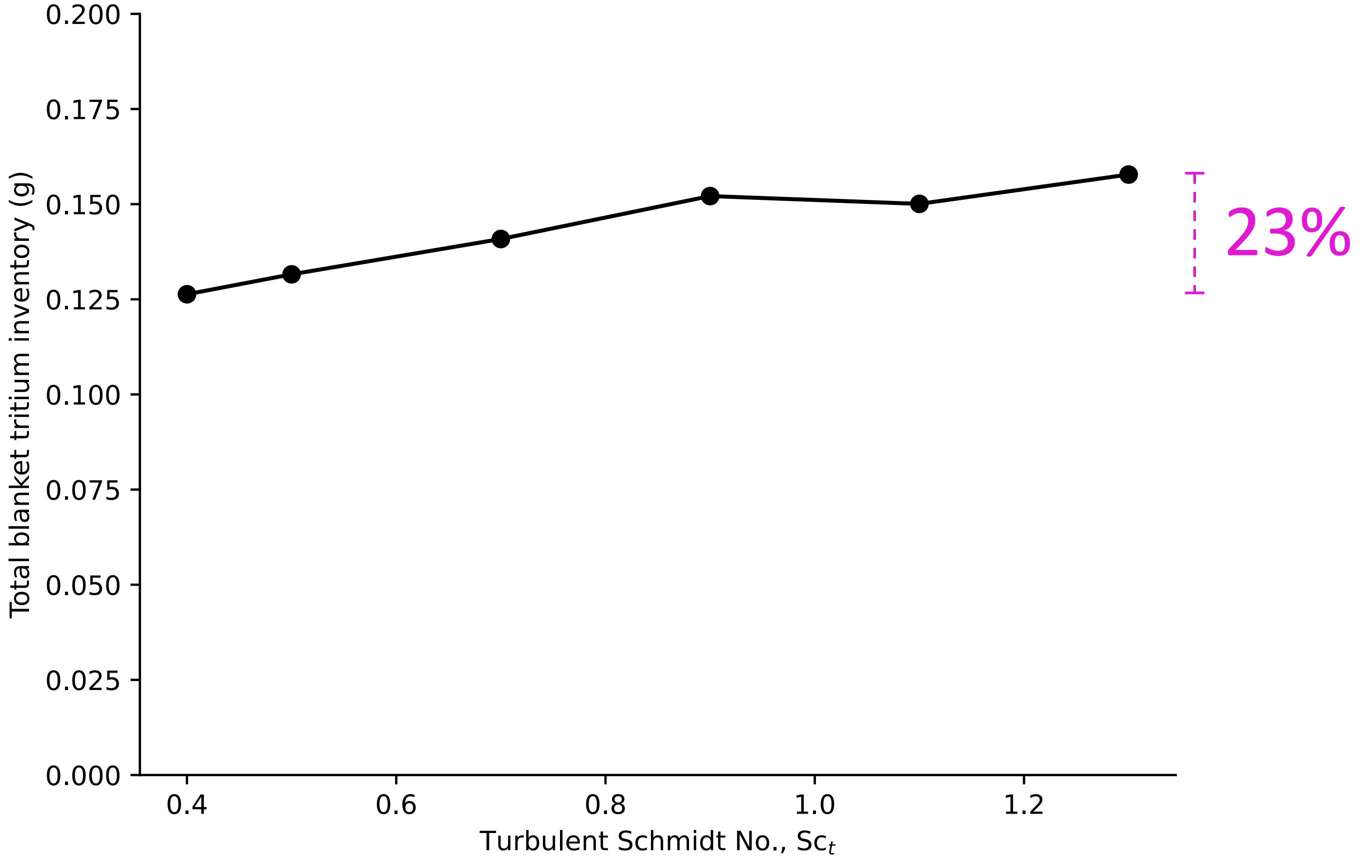
- Can use transient data to parametrise system code
- Tritium extraction systems will deal with constantly changing concentrations
  - But extraction efficiency scales with tritium concentration
  - **Needs to be accounted for in the design process**

Parametric study: Influence of $\mathrm{Sc_t}$

$$D_{\mathrm{turb}} = \frac{\nu_t}{\mathbf{Sc}_t}$$

Turbulent diffusion affects the concentration field.

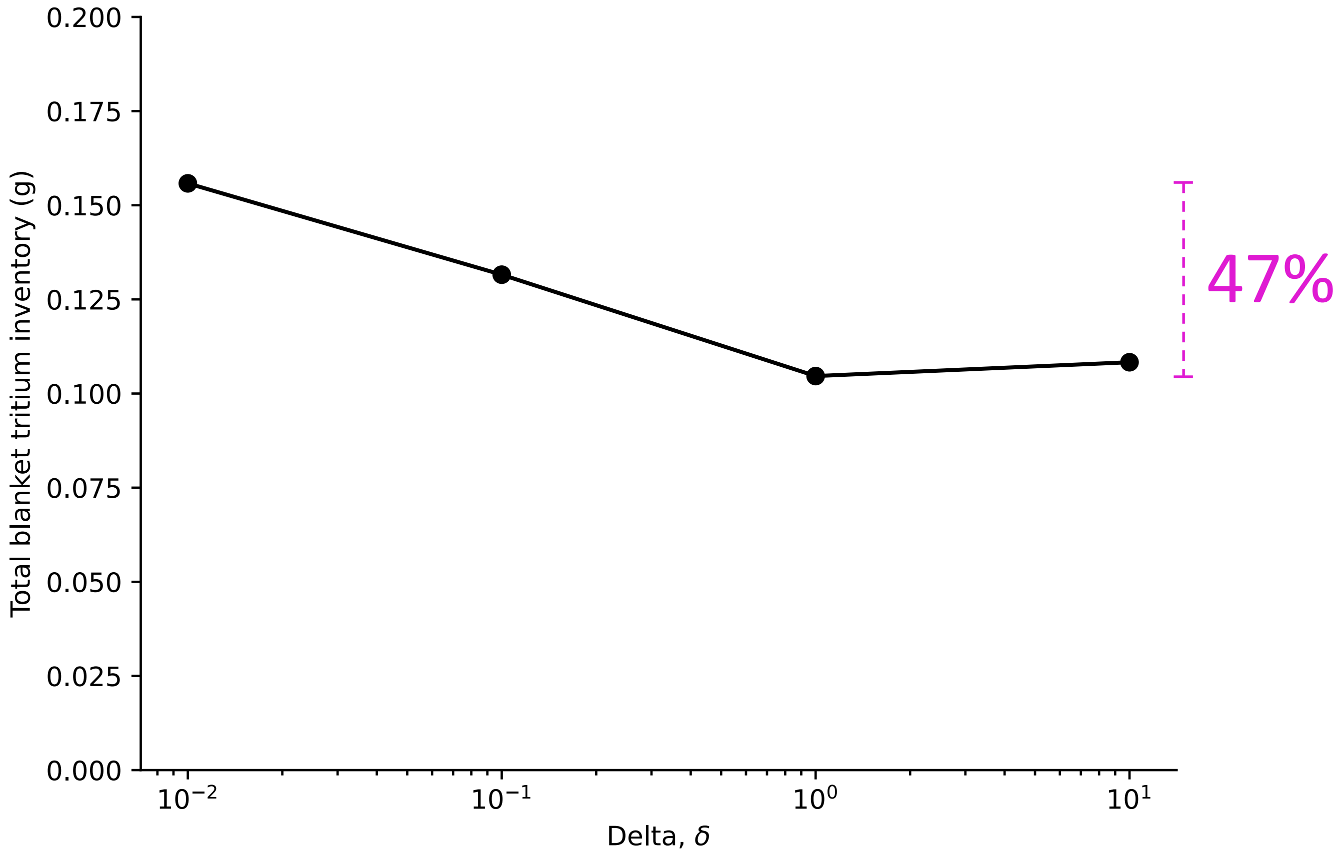
But unclear what Schmidt number should be used.



Parametric study: Influence of artificial diffusion

$$D_{\text{art}} = \boldsymbol{\delta} h||u||$$

- Used to help converge
- The lower, the better
- The mesh could do some more refinement



ARC blanket: How to take it further?

Physics & modelling enhancements

- More detailed geometry
- Add trapping effects
- Non-zero inlet concentration (extraction efficiency)
- First wall implantation from plasma

Chemistry & Reactions

- Chemical reactions
- Redox potential
- Speciation

Methodology & Validation

- Uncertainty quantification
- Leakage out of the vessel
- Integrate with system-level codes

Conclusion

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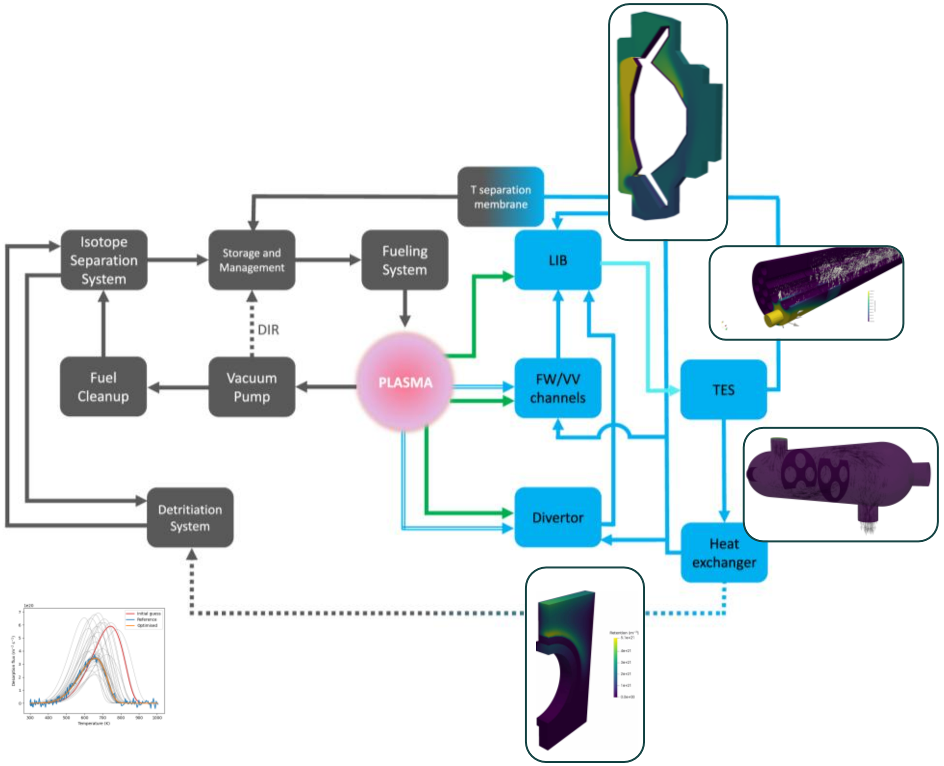

- Looking to submit this work in a publication soon!
- Looking to do more detailed models on different components of the tritium fuel cycle.

Source code Tutorials V&V book

Contact: **darkj385@mit.edu**

Back-up Slides

Hydrogen transport equations

$$\frac{\partial c_m}{\partial t} = \overbrace{\nabla \cdot (D \nabla c_m)}^{\text{Diffusion}} + \overbrace{S}^{\text{Source}} + \overbrace{u \nabla c_m}^{\text{Advection}} - \overbrace{\sum \frac{\partial c_{t,i}}{\partial t}}^{\text{Trapping}}$$

$$\frac{\partial c_{\mathrm{t},i}}{\partial t} = \underbrace{\nu_{t,i}}_{\substack{\text{Trapping}\\ \text{rate}}} c_{\mathrm{m}} \underbrace{\left(n_i - c_{\mathrm{t},i}\right)}_{\substack{\text{Free}\\ \text{traps}}} - \underbrace{\nu_{dt,i}}_{\substack{\text{De-trapping}\\ \text{rate}}} c_{\mathrm{t},i}$$

Meet the team

Maintainers

Rémi Delaporte-Mathurin

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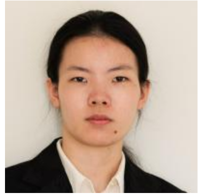
James Dark

MIT, USA

Vladimir Kulagin

MEPhI, Russia

MIT team



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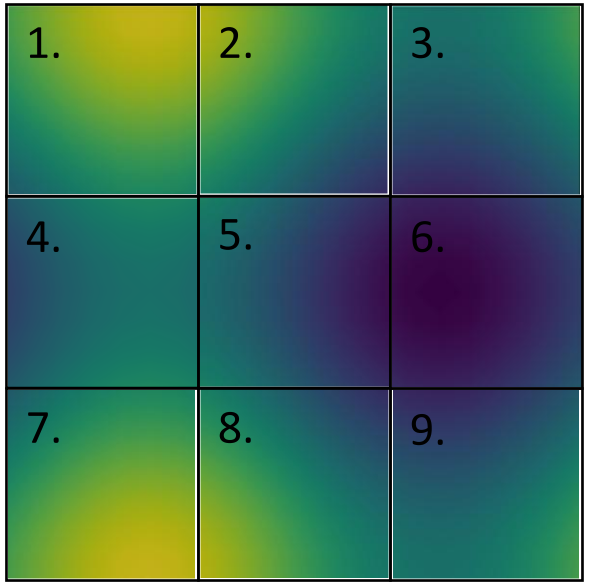
Samuele Meschini

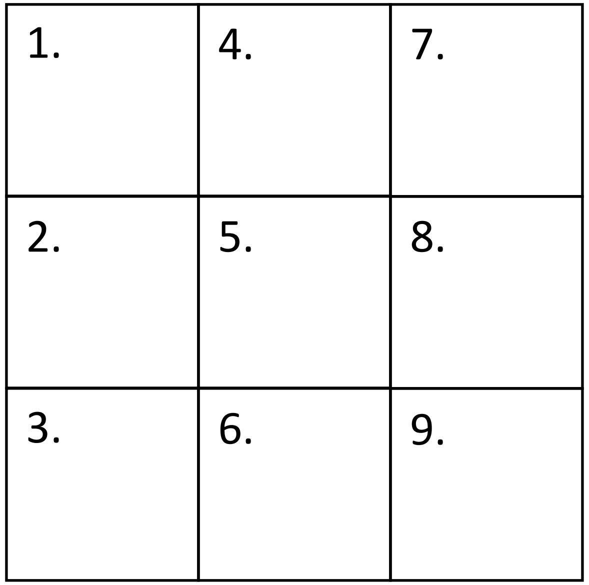
Polito, Italy

Openmc2dolfinx and foam2dolfinx

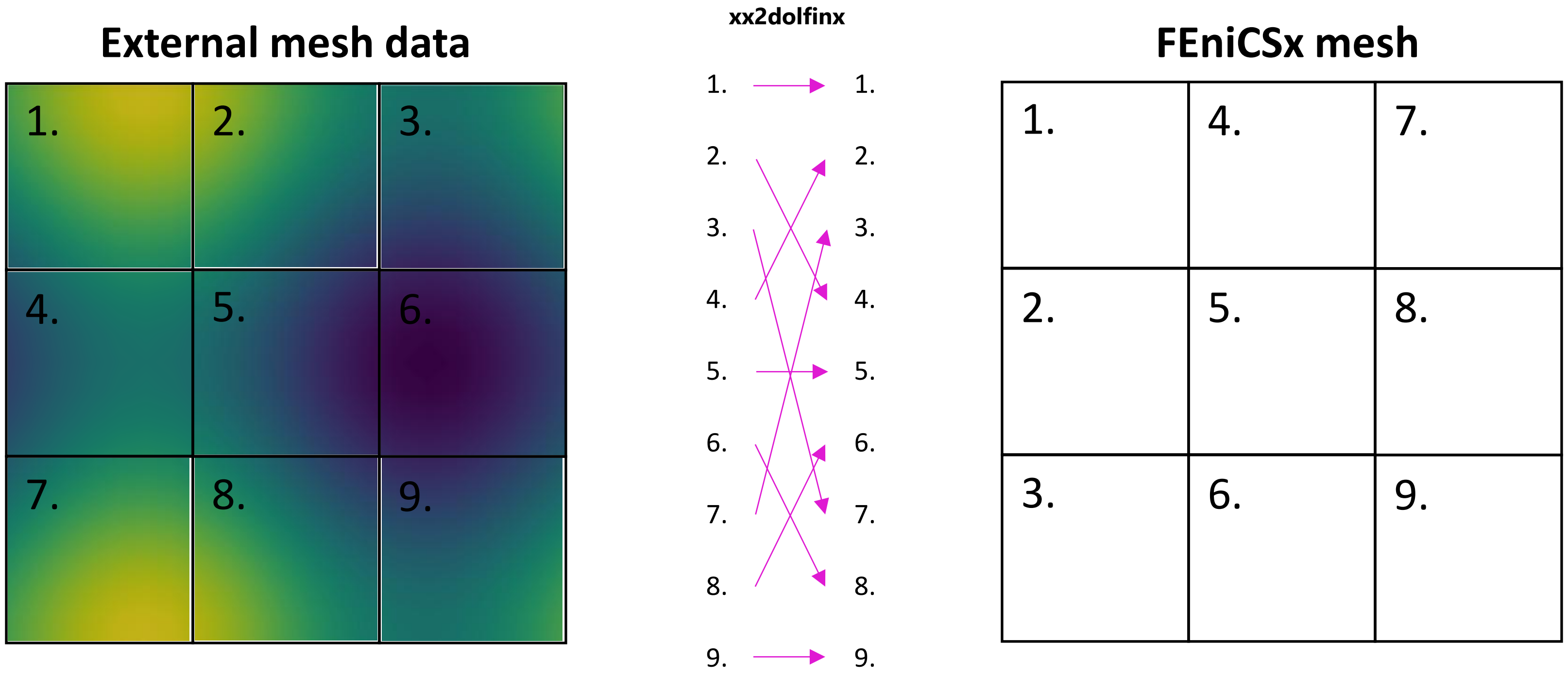
External mesh data



FEniCSx mesh

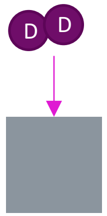


Openmc2dolfinx and foam2dolfinx

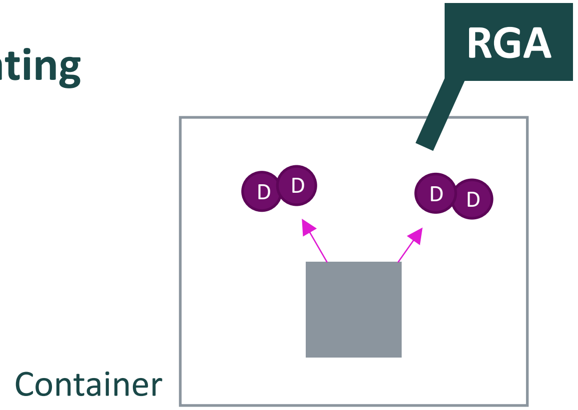


Modelling TDS experiments

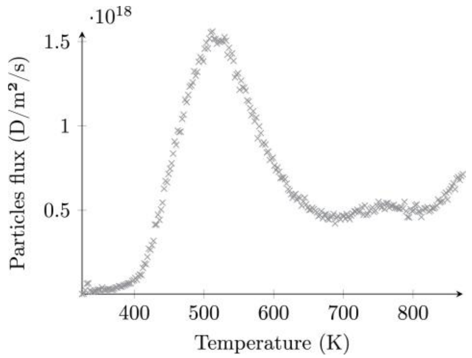
1. Implantation



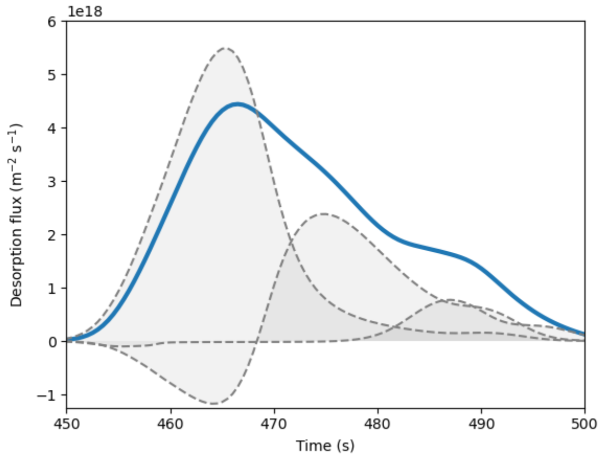
2. Heating



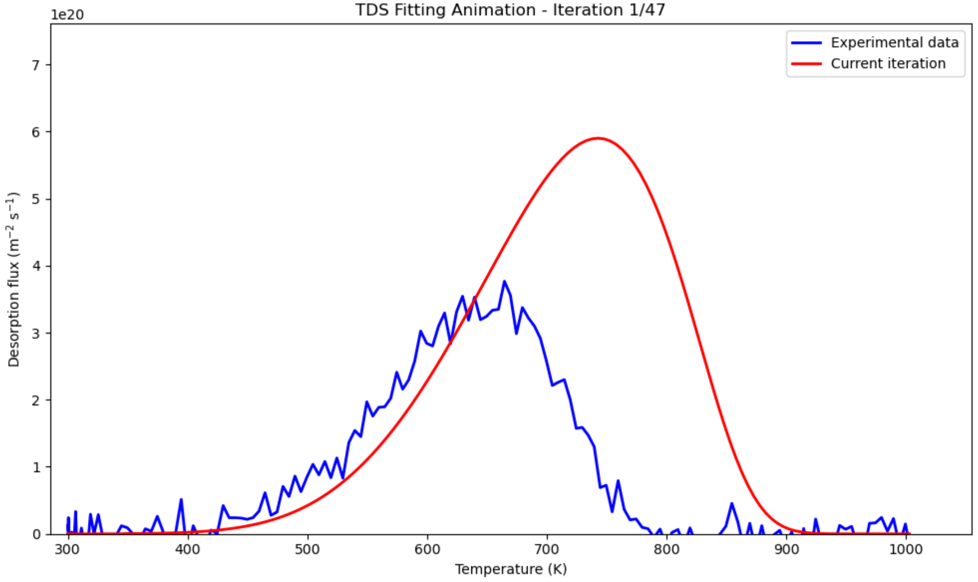
3. Measure desorption



With FESTIM:



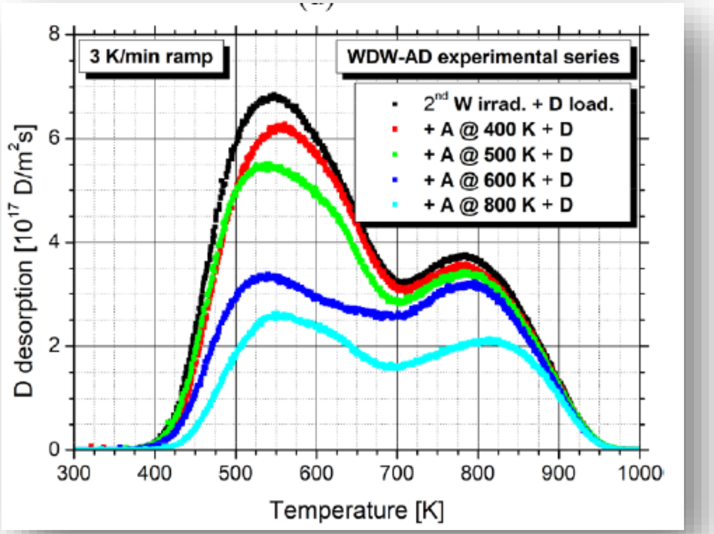
Integrate with external tools for automated fitting:



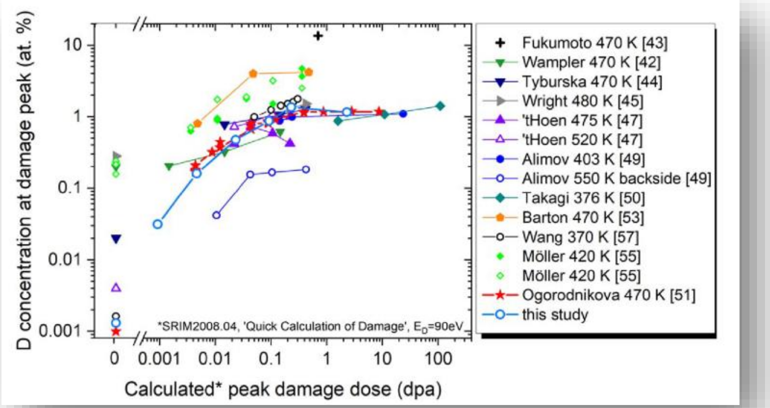
Damage-induced traps

- Neutron damage will induce defects in structural materials

- Literature shows temperature dependence and saturation in tritium retention



M. Pečovnik (2020) 10.1088/1741-4326/ab680f



T. Schwartz-Selinger (2024) 10.1088/2053-1591/acfdf8

Damage-induced traps

trap density
[m^{-3}]

Creation from damage — Destruction by annealing

$$\frac{\partial n_t}{dt} = \phi \cdot K \left[1 - \frac{n_t}{n_{\max,\phi}}\right] - A \cdot n_t$$

damage rate
[dpa s^{-1}]

trap creation factor
[m^{-3} dpa^{-1}]

maximum trap density
[m^{-3}]

trap annealing factor
[s^{-1}]

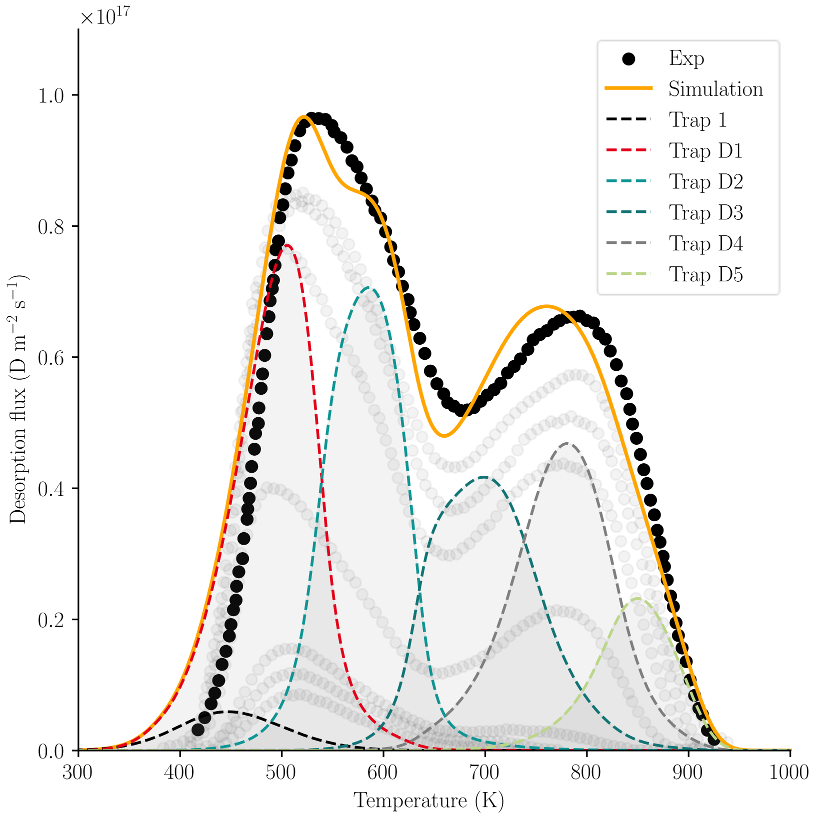
Damage-induced traps

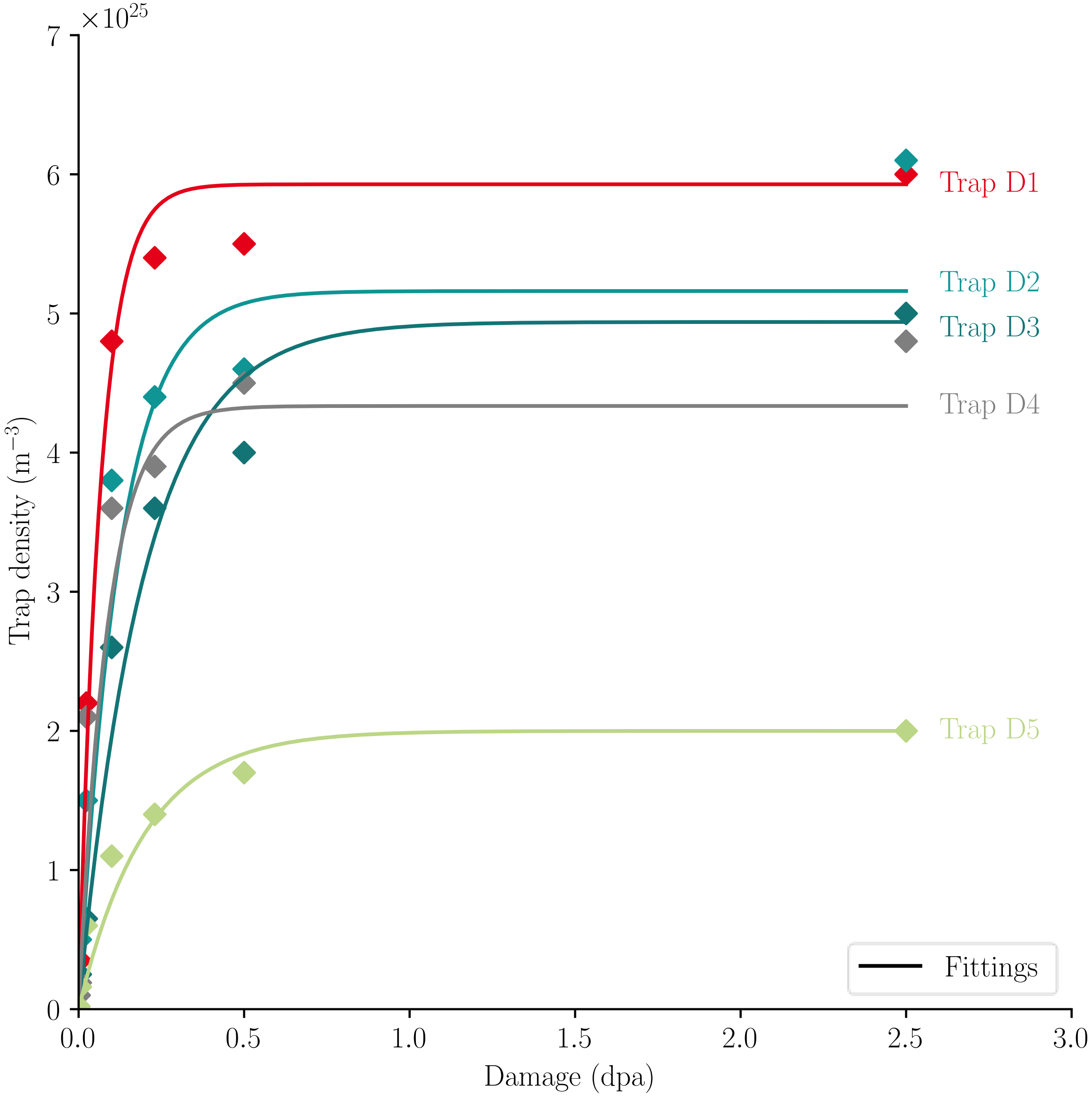
- Self-damaged W samples used in TDS experiments fitted with extrinsic traps

- Trap density evolution fitted using current model

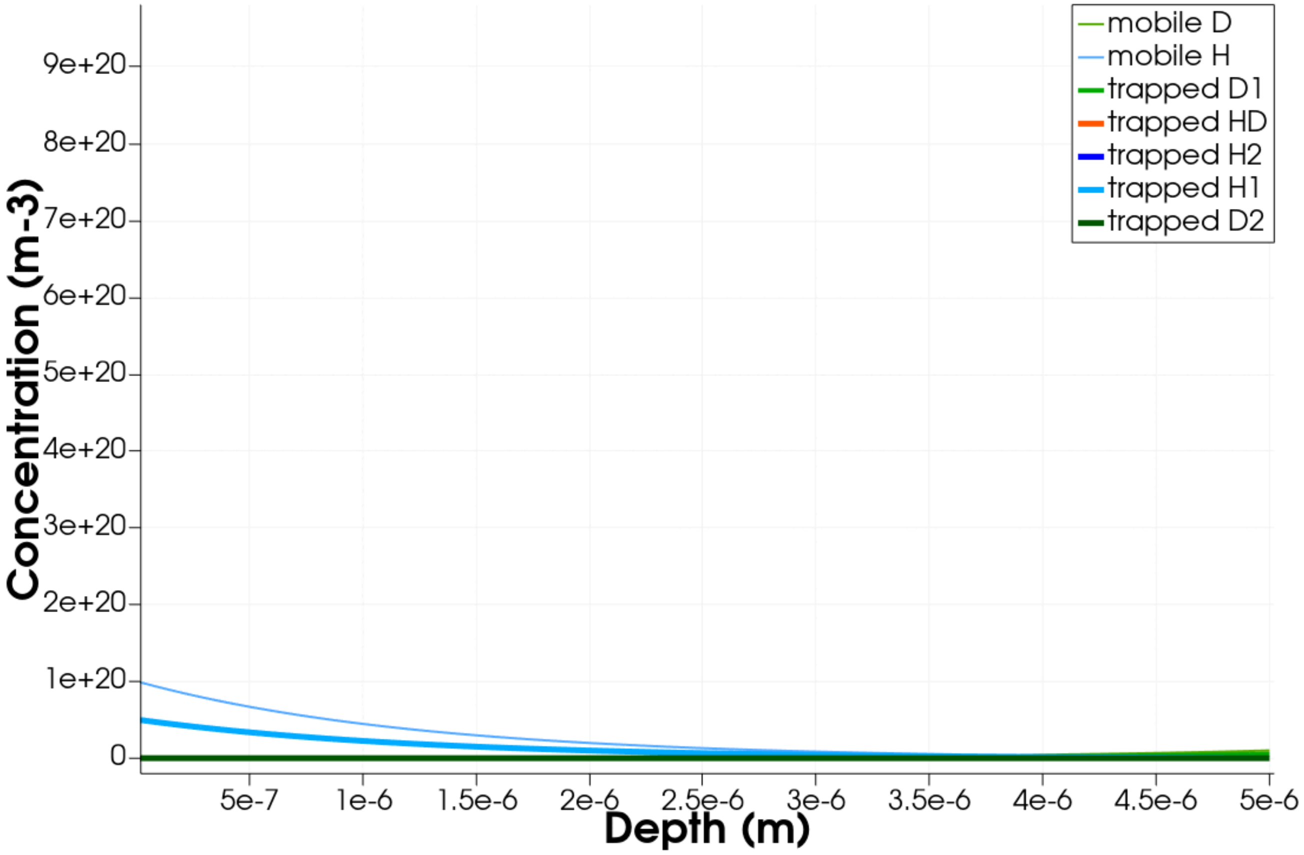
2.5
0.5
0.23
0.1
0.023
0.005
0.001

DPA



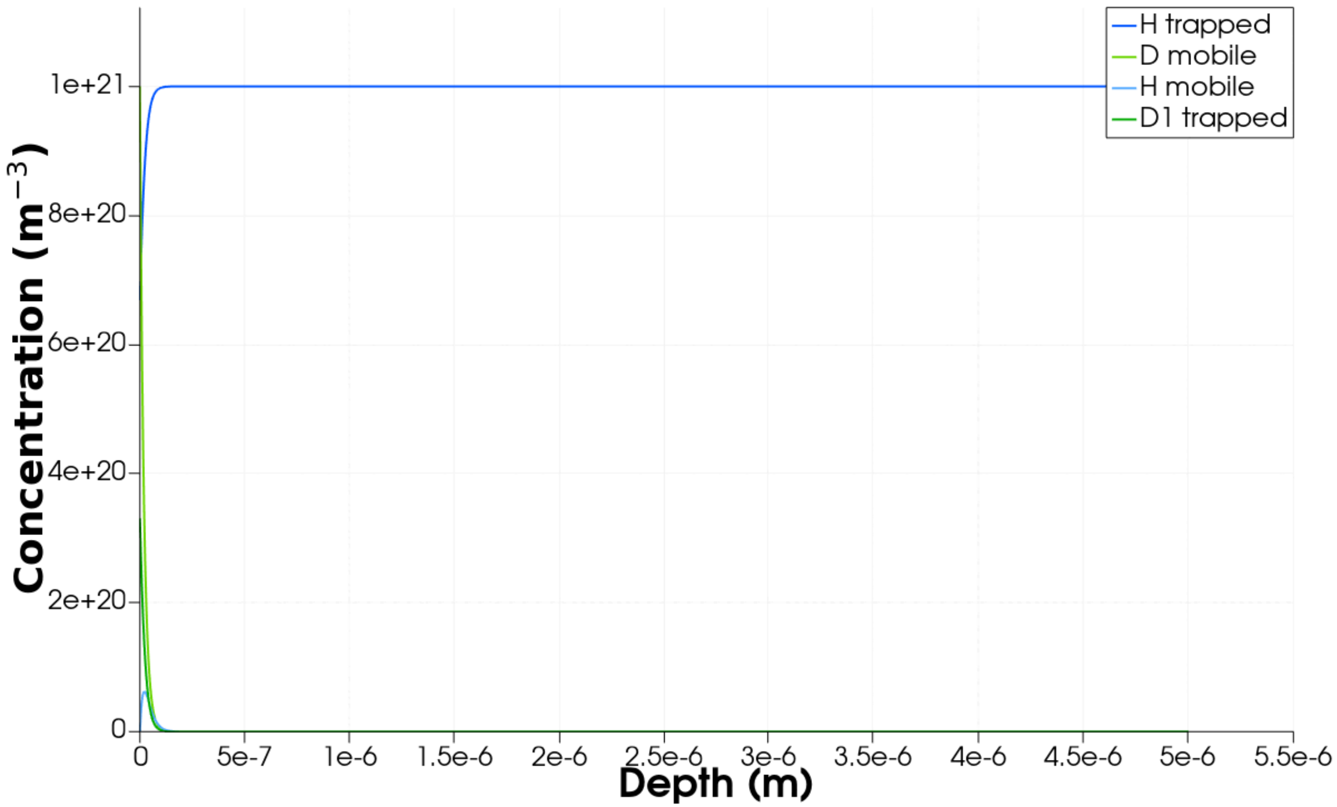


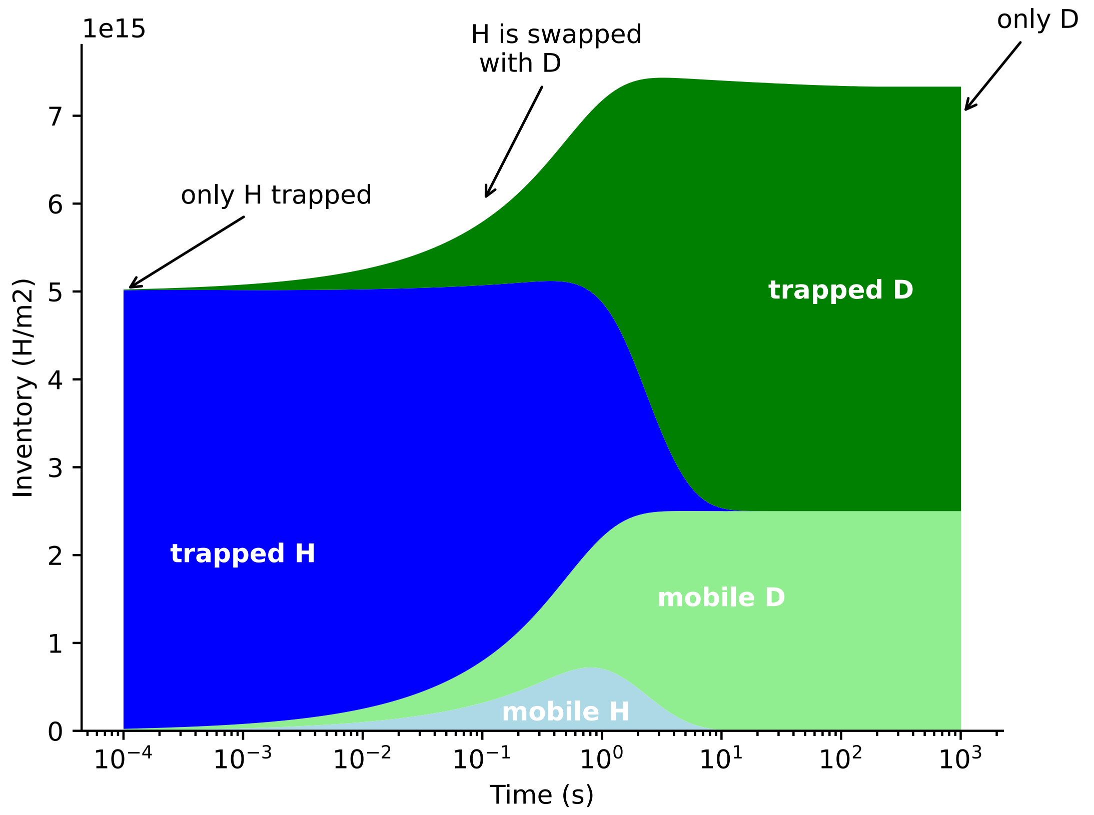
Multi-isotope, multi-level trapping



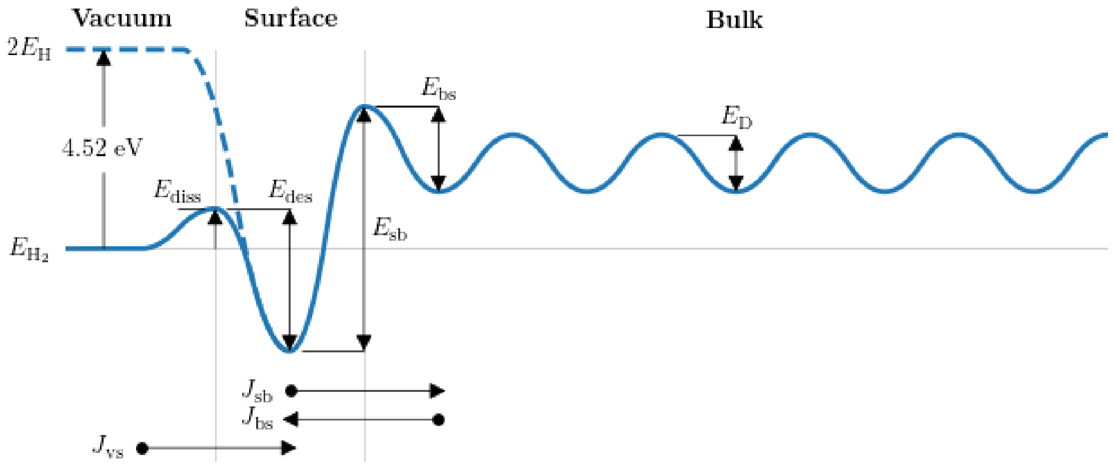
- 7 different species
- 6 reactions
- $c_H = 10^{20}\ \mathrm{m}^{-3}$ on the left
- $c_D = 10^{19}\ \mathrm{m}^{-3}$ on the right

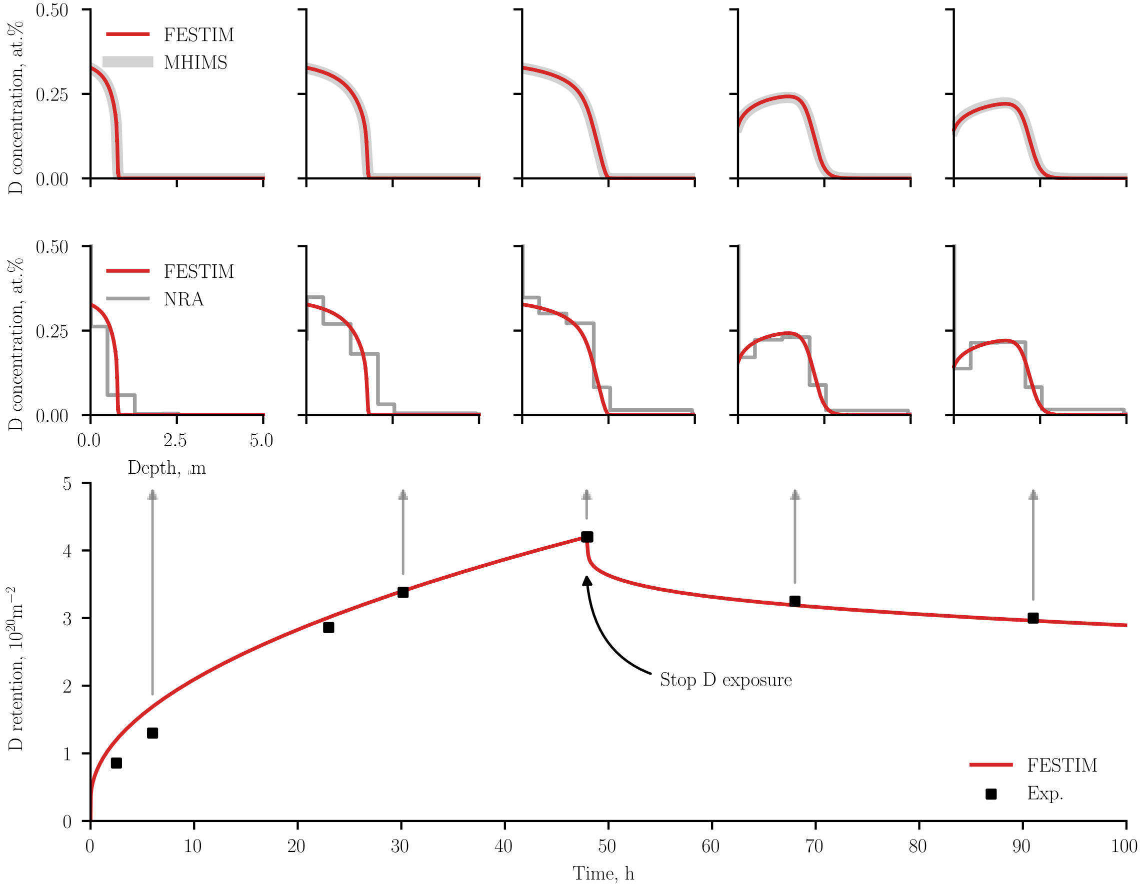
Isotope swapping





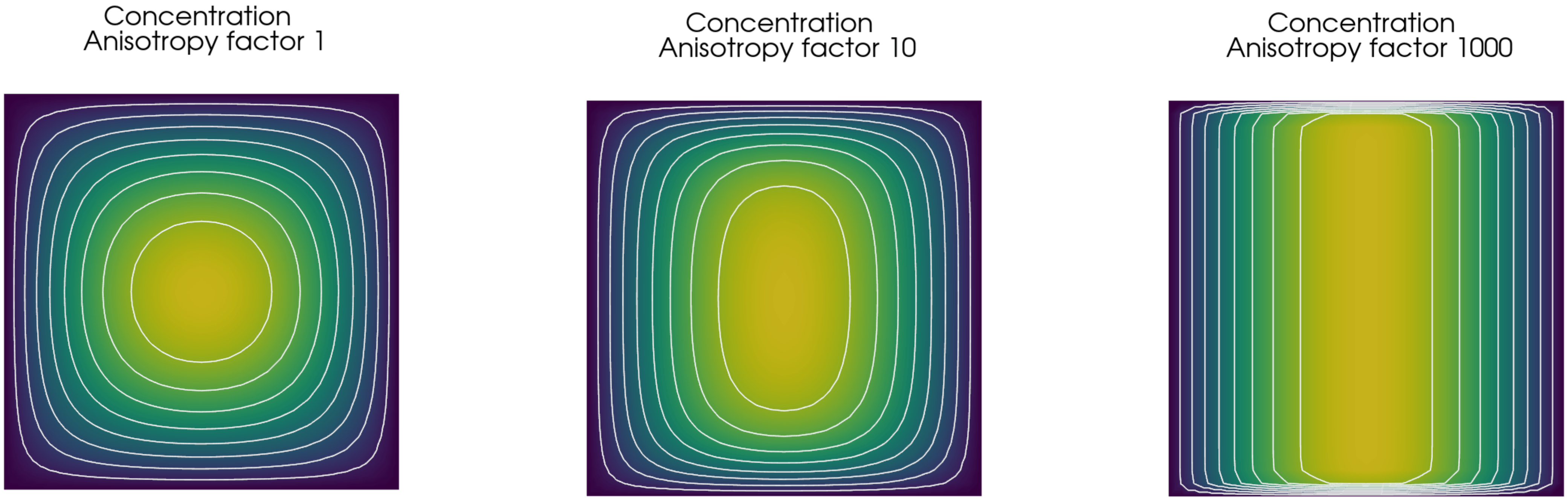
Kinetic surface model





- D in damaged W (S. Markelk JNM 2016)
- Comparison with NRA profiles

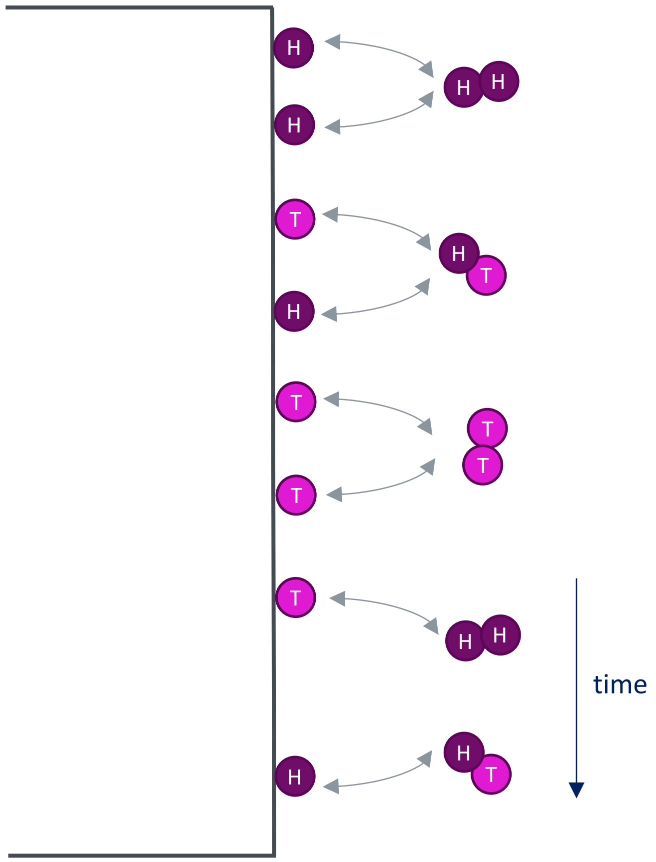
Anisotropy



$$D = \begin{bmatrix} D_{xx} & 0 \\ 0 & D_{yy} \end{bmatrix}$$

- Anisotropic materials can be simulations with very few modifications
- Composites
- Anisotropic microstructures

Surface Reactions



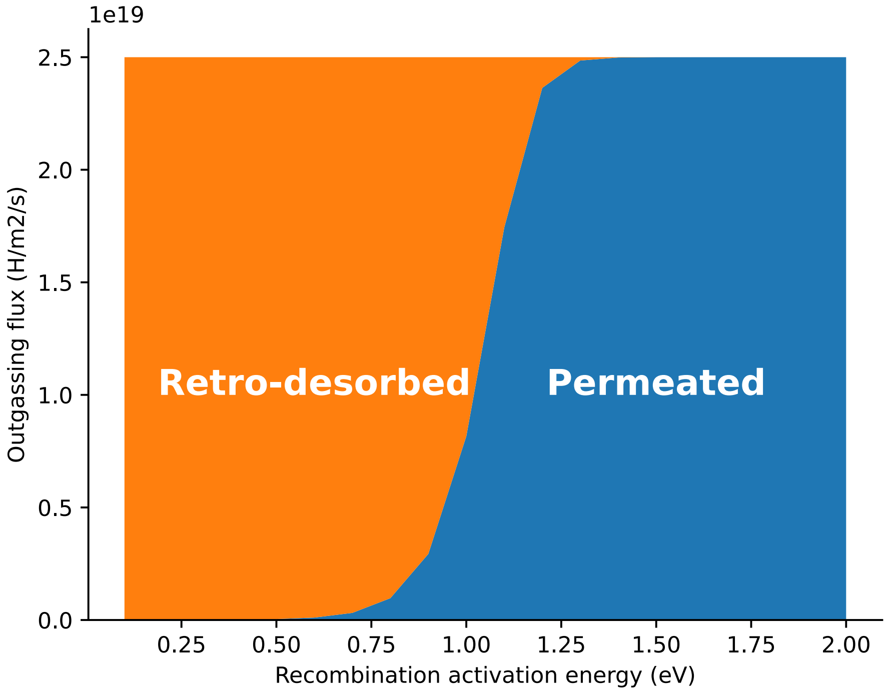
$$H + H \underset{p_i}{\overset{k_i}{\leftrightarrow}} H_2$$

$$H + T \underset{p_i}{\overset{k_i}{\leftrightarrow}} HT$$

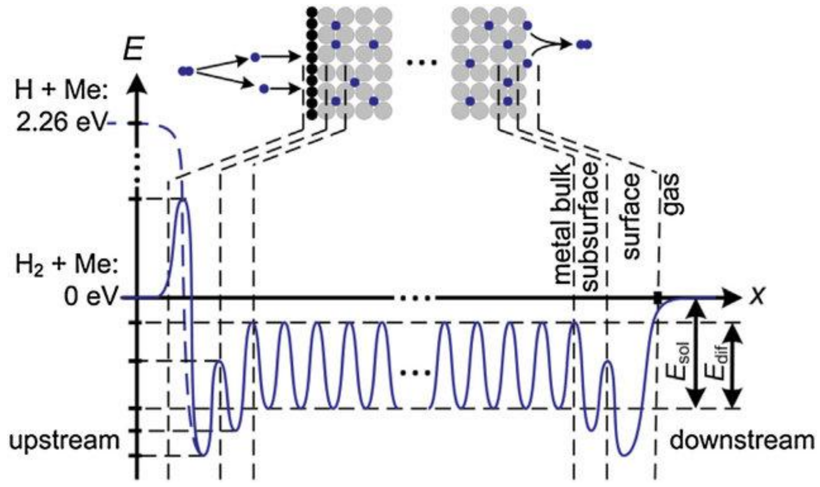
$$T + T \underset{p_i}{\overset{k_i}{\leftrightarrow}} T_2$$

$$T + H_2 \underset{p_i}{\overset{k_i}{\leftrightarrow}} HT + H$$

Metal foil pumps for DIR



- H is implanted in first 10 nm
- Super-permeation regime is attained at high-recombination energy (upstream surface)



Benedikt & Day, (2017) Fusion Engineering and Design

FESTIM is verified & validated

festim-vv-report.readthedocs.io

FESTIM V&V online book [1]

Verified against complex analytical solutions

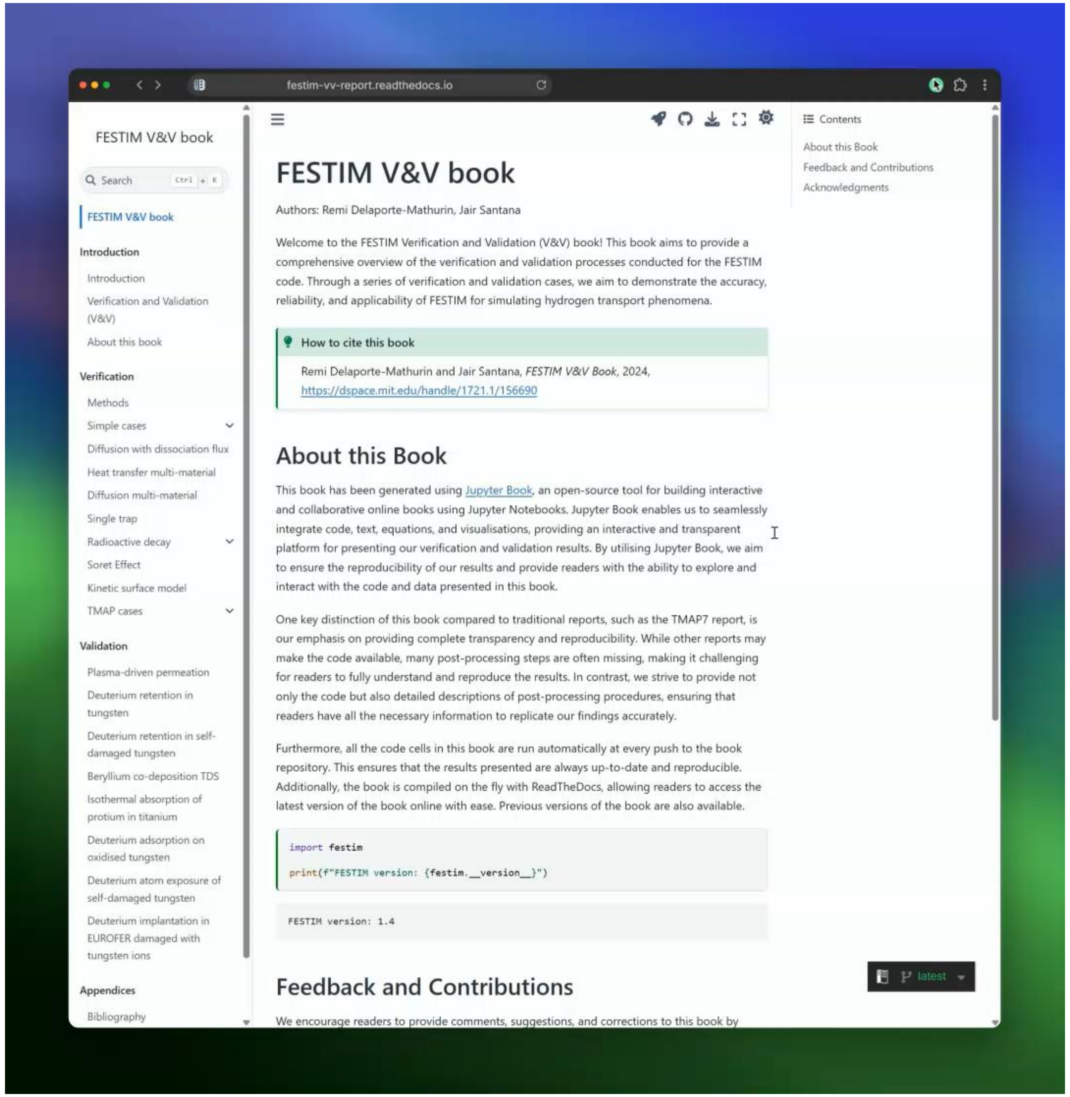
- Tested in 1/2/3D

Validated against experimental data

✅ Scripts available - including pre/post processing

✅ Live - can run, update and edit

✅ Version control - each version citable



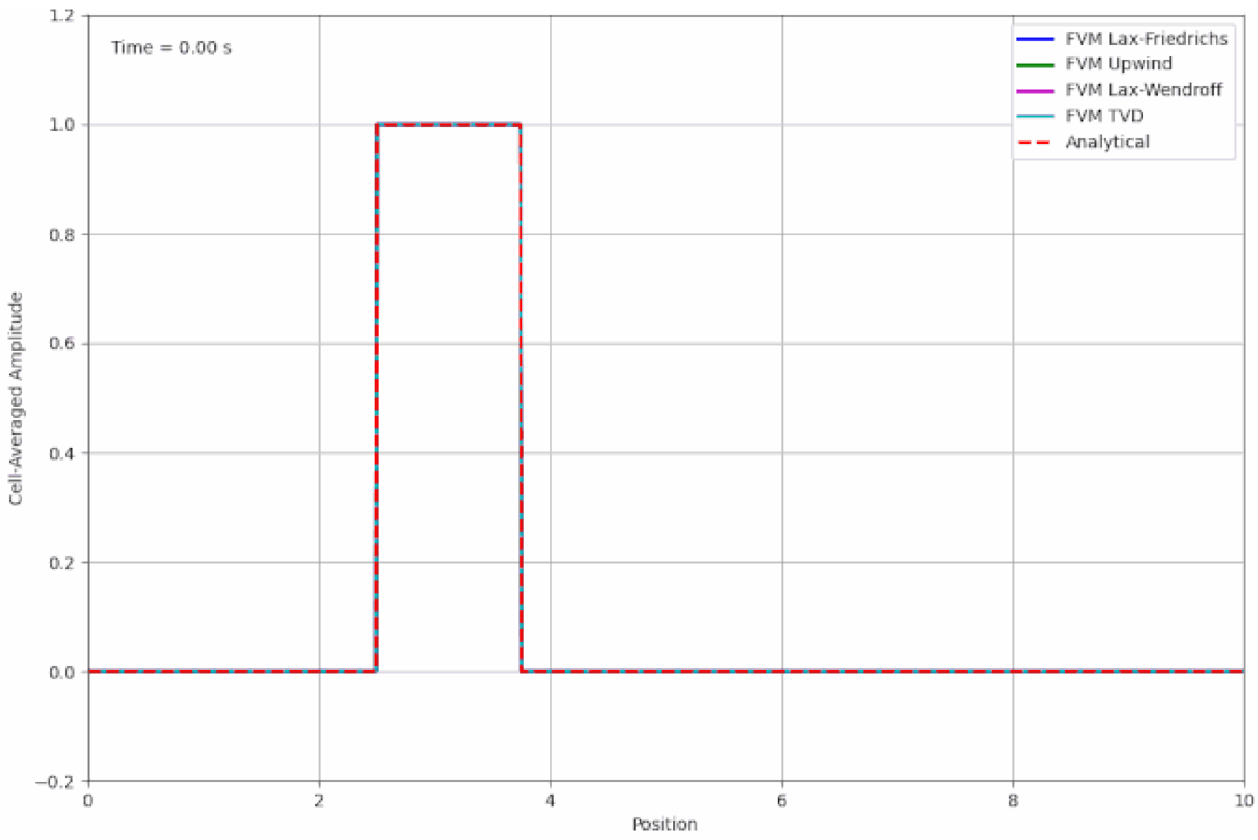
[1] - R. Delaporte-Mathurin & J. Santana, *FESTIM V&V book, v3,* (2024), dspace.mit.edu/handle/1721.1/156690.

Artificial diffusion stabilization

Problem with advection diffusion problems in FEM

Can reduce this error by:

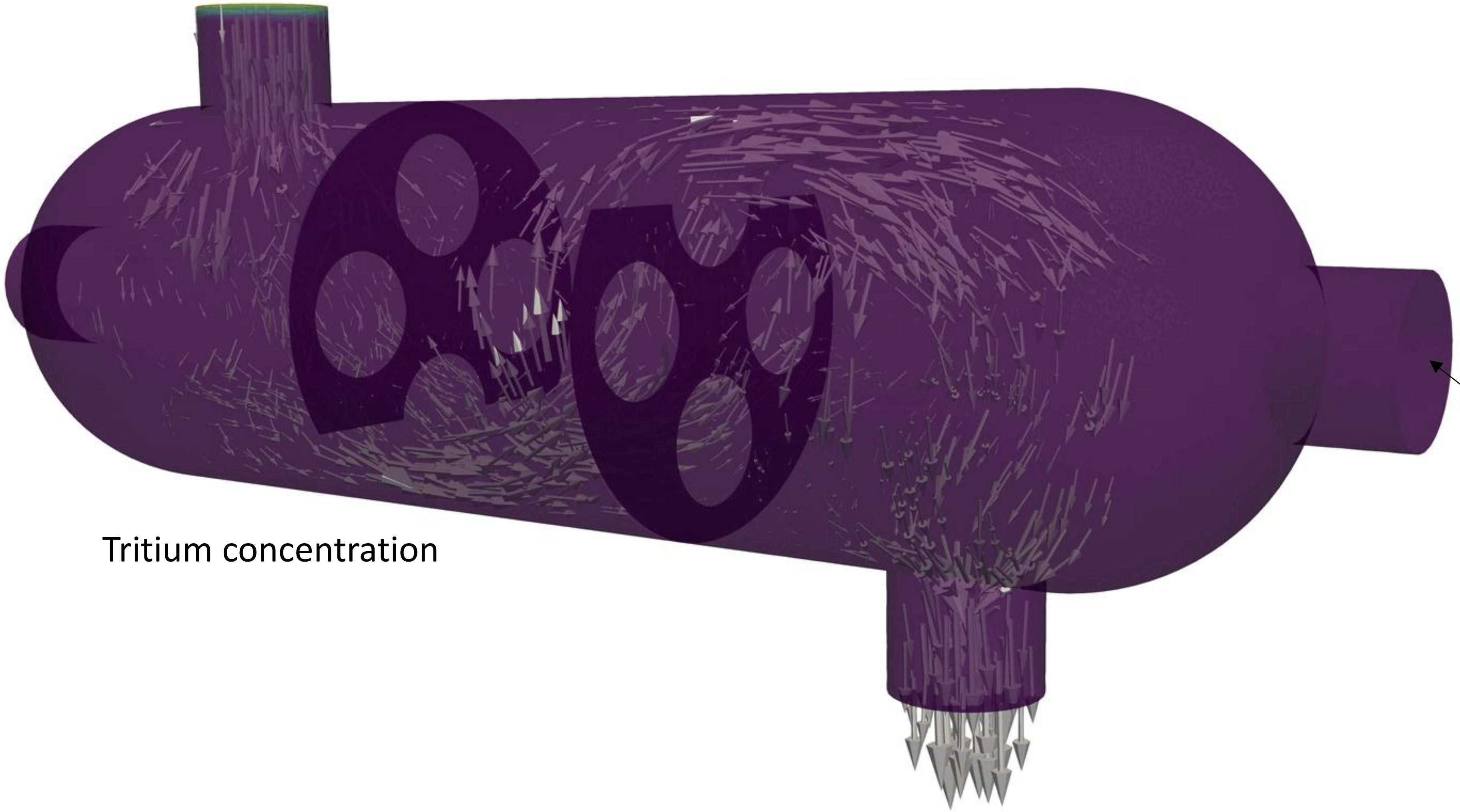
- Reduce time step
- Increase mesh refinement
- Use stabilisers
- Use alternate solver



Heat exchanger and extraction systems

OpenFOAM

Coupling **FESTIM** with **CFD codes**



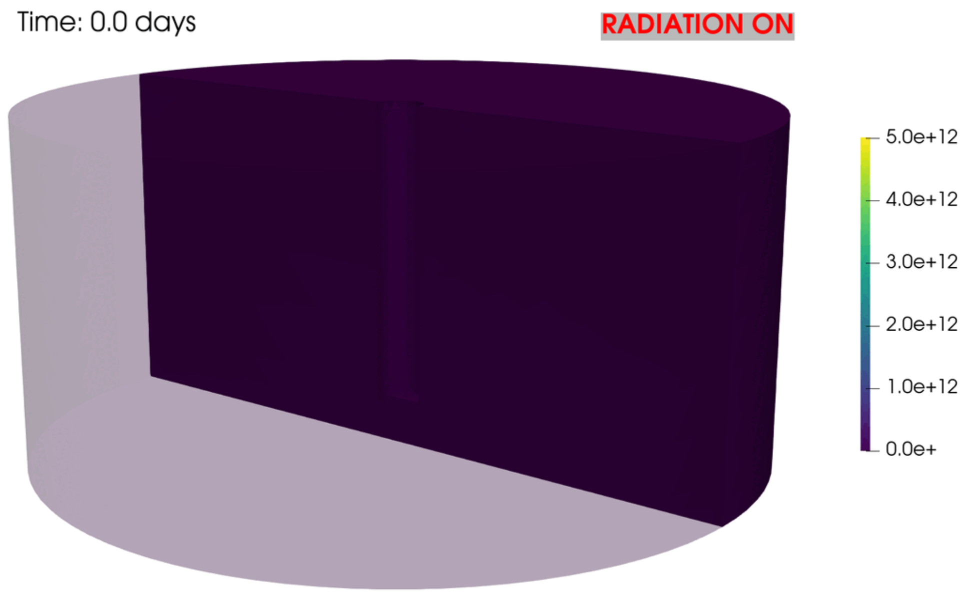
Tritium concentration

Tritium coming out from hot outlet

Breeding blanket technology

LIBRA

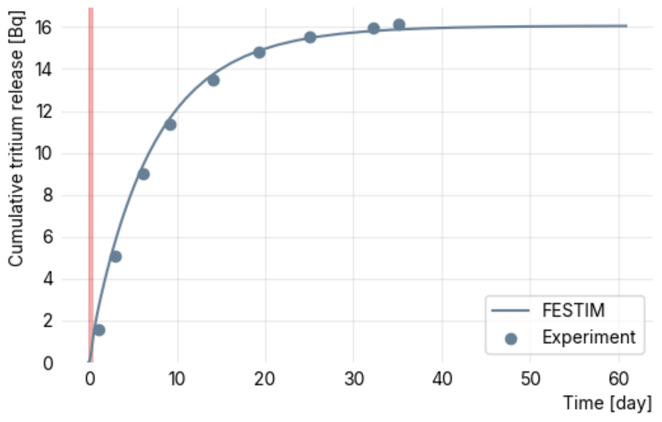
Coupling with FESTIM with neutronics codes



OpenMC

Tritium concentration (m^{-3})

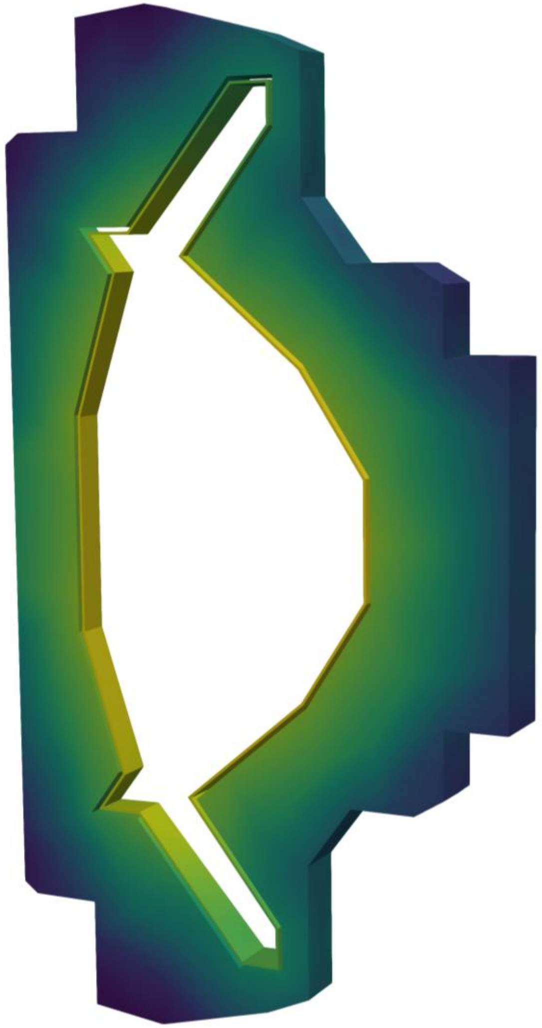
Good agreement with experimental data



Serves as a multi-physics validation case

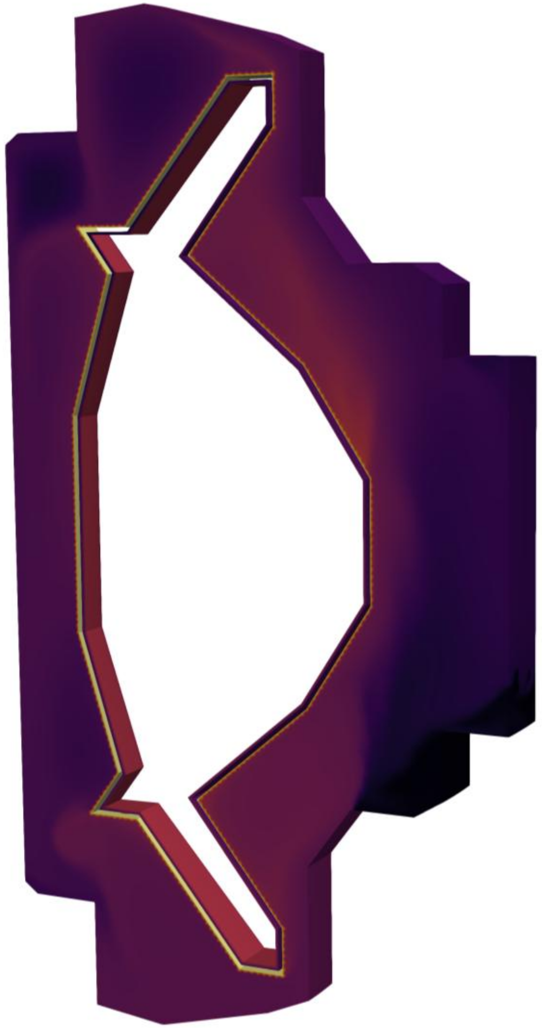
ARC OpenMC results

Nuclear heating

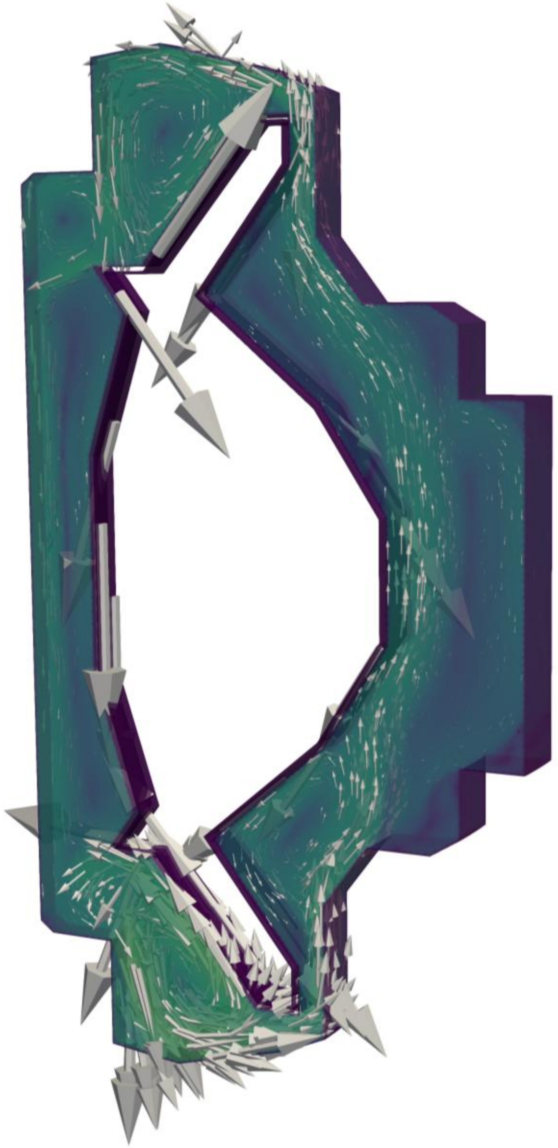


Tritium generation

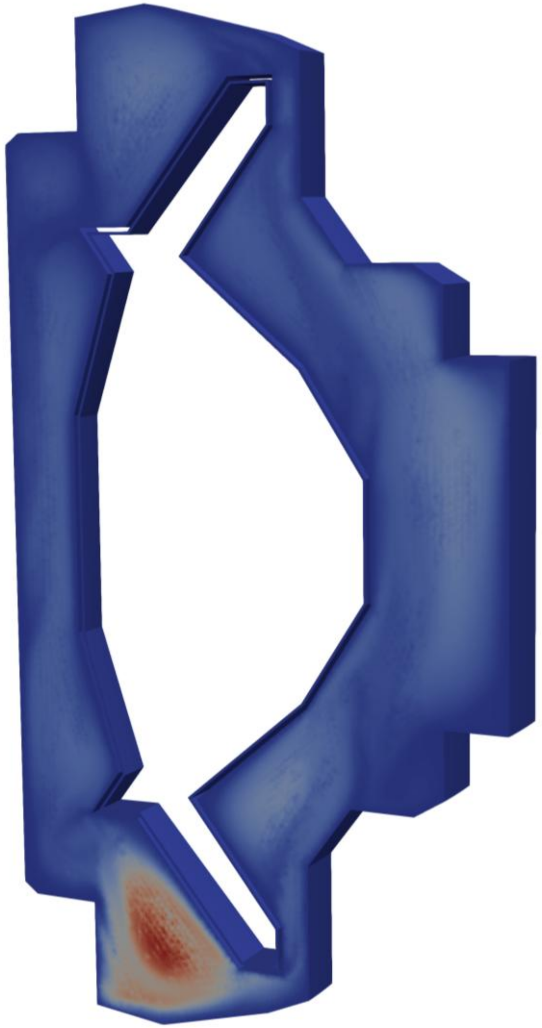
ARC OpenFOAM results



Temperature



Velocity

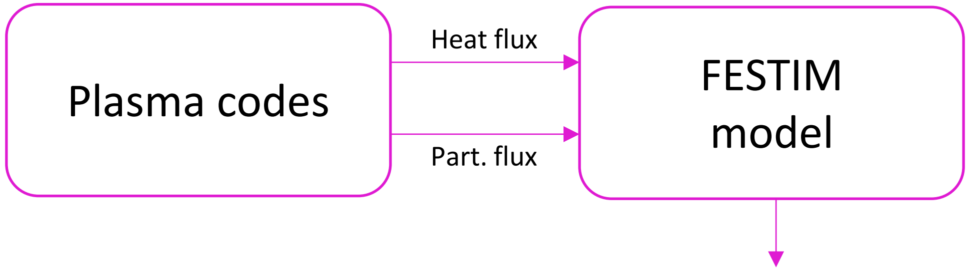


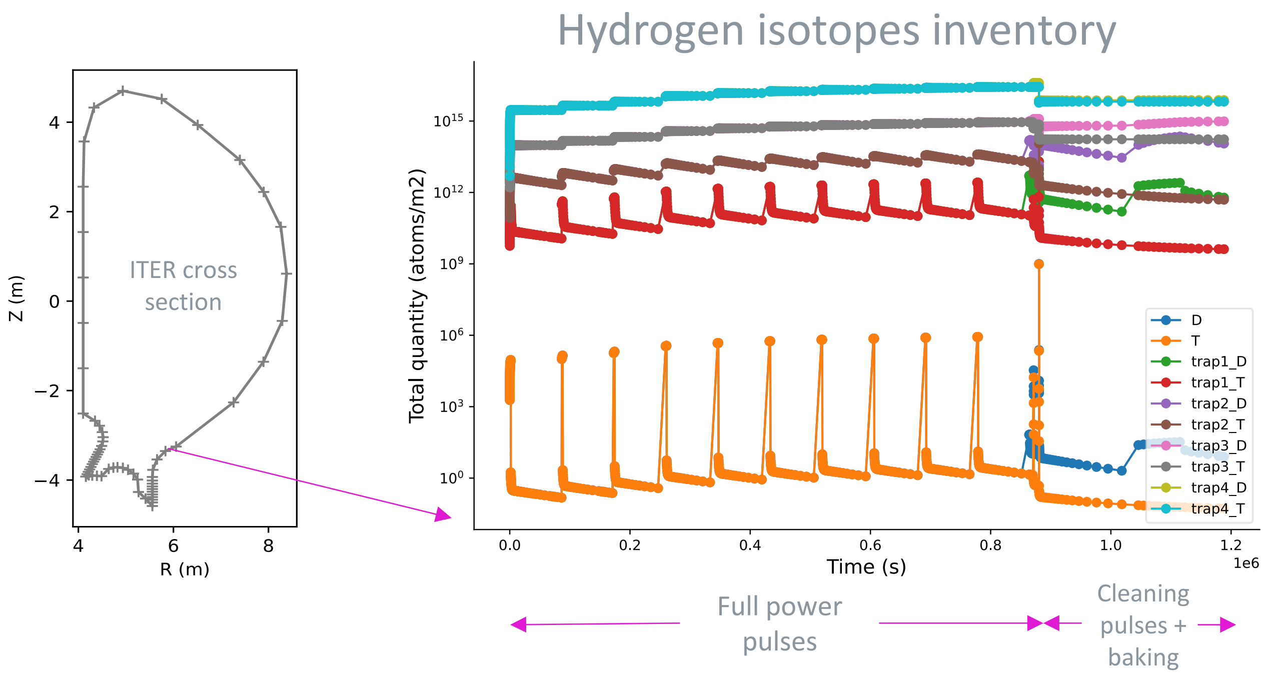
Turbulent
viscosity

HISP: coupling FESTIM to plasma codes

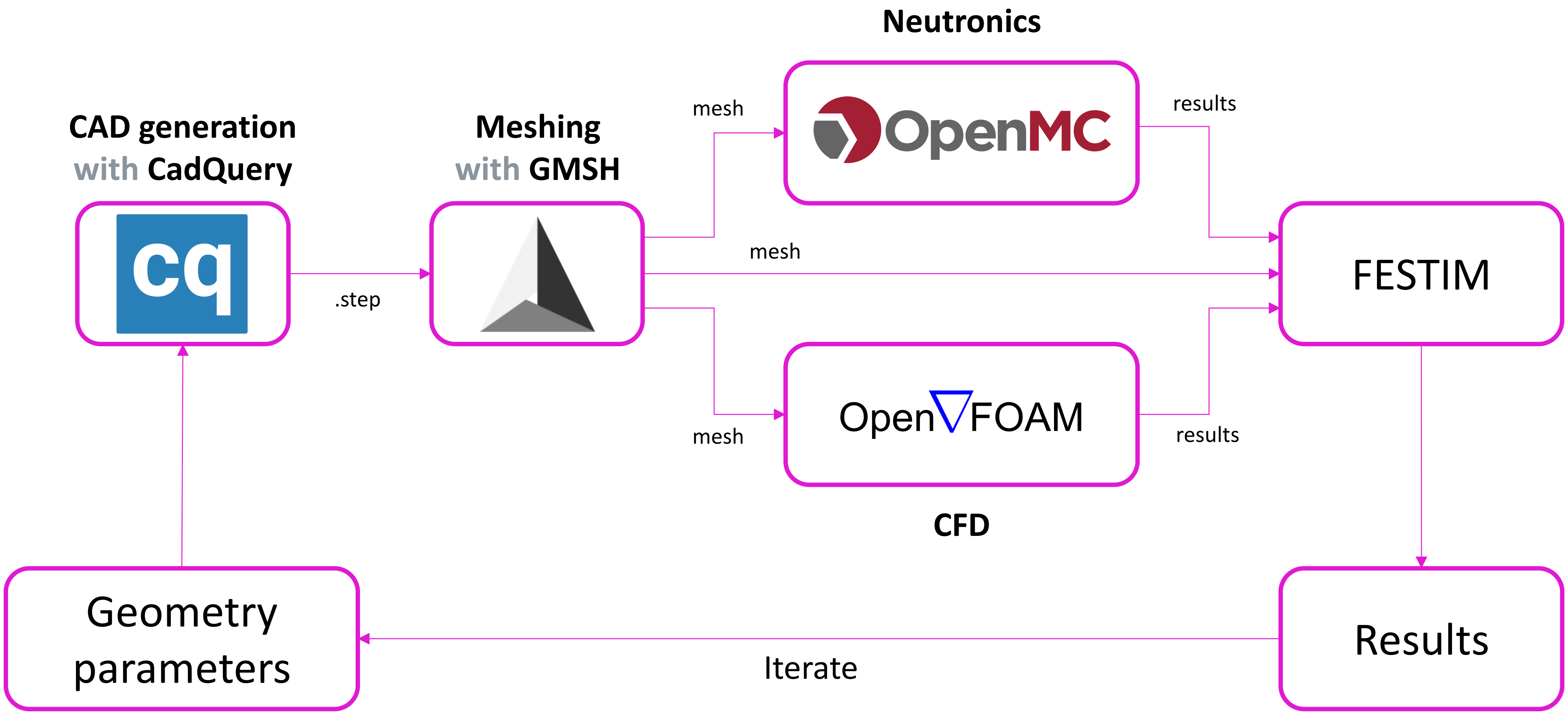
- Tracks **deuterium** and **tritium** in PFC's
- Interfaces plasma codes (DINA, SMITER, SOLEDGE, SOLPS…) to FESTIM
- Used to inform **ITER PFC's de-tritiation** strategies
- Built to be **reactor-agnostic** and **plasma-code agnostic**

github.com/festim-dev/hisp

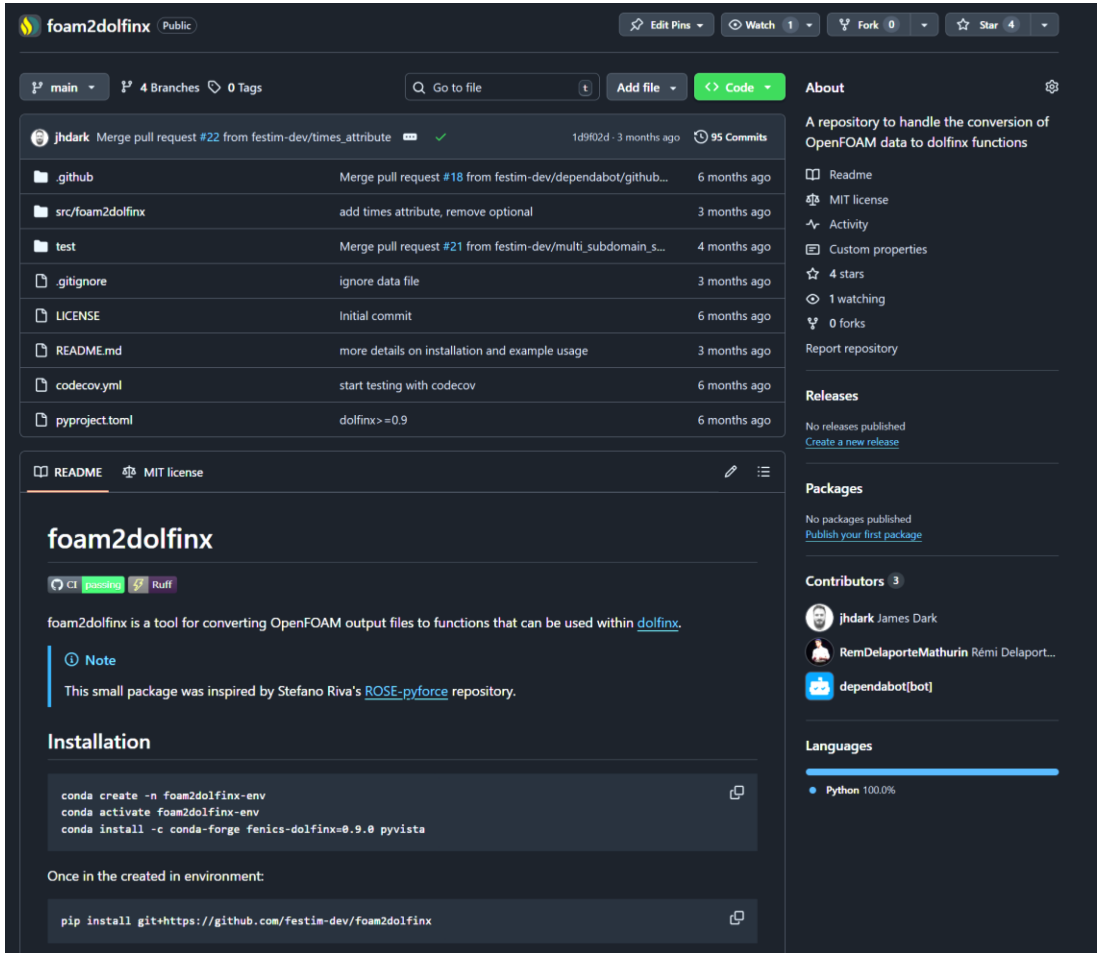


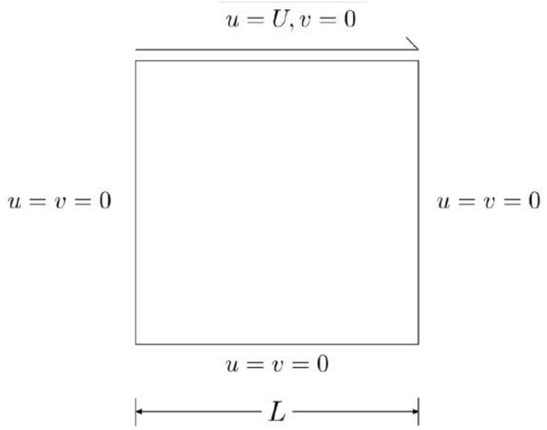


Open-source iterative design workflow

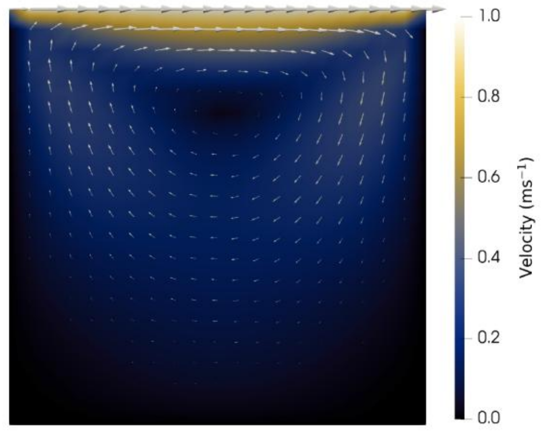


foam2dolfinx

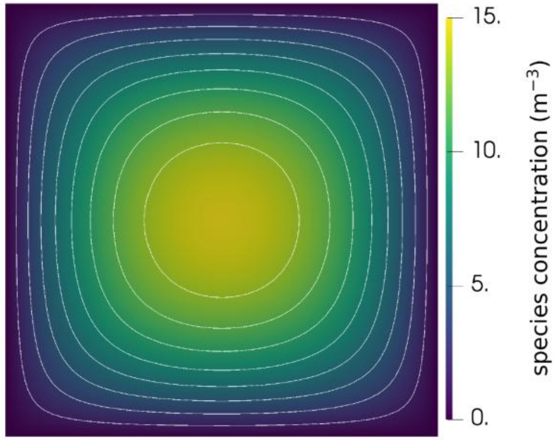




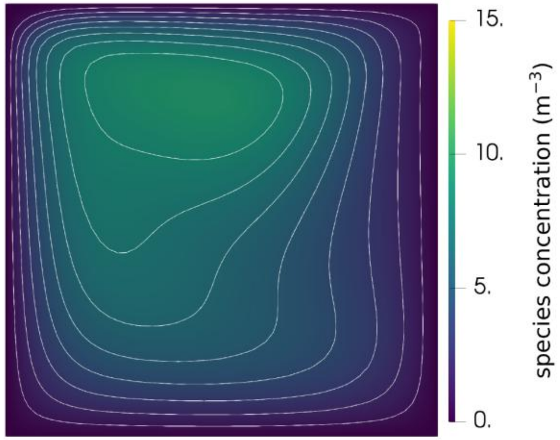
(a) Lid-driven cavity problem setup



(b) Velocity field from OpenFOAM

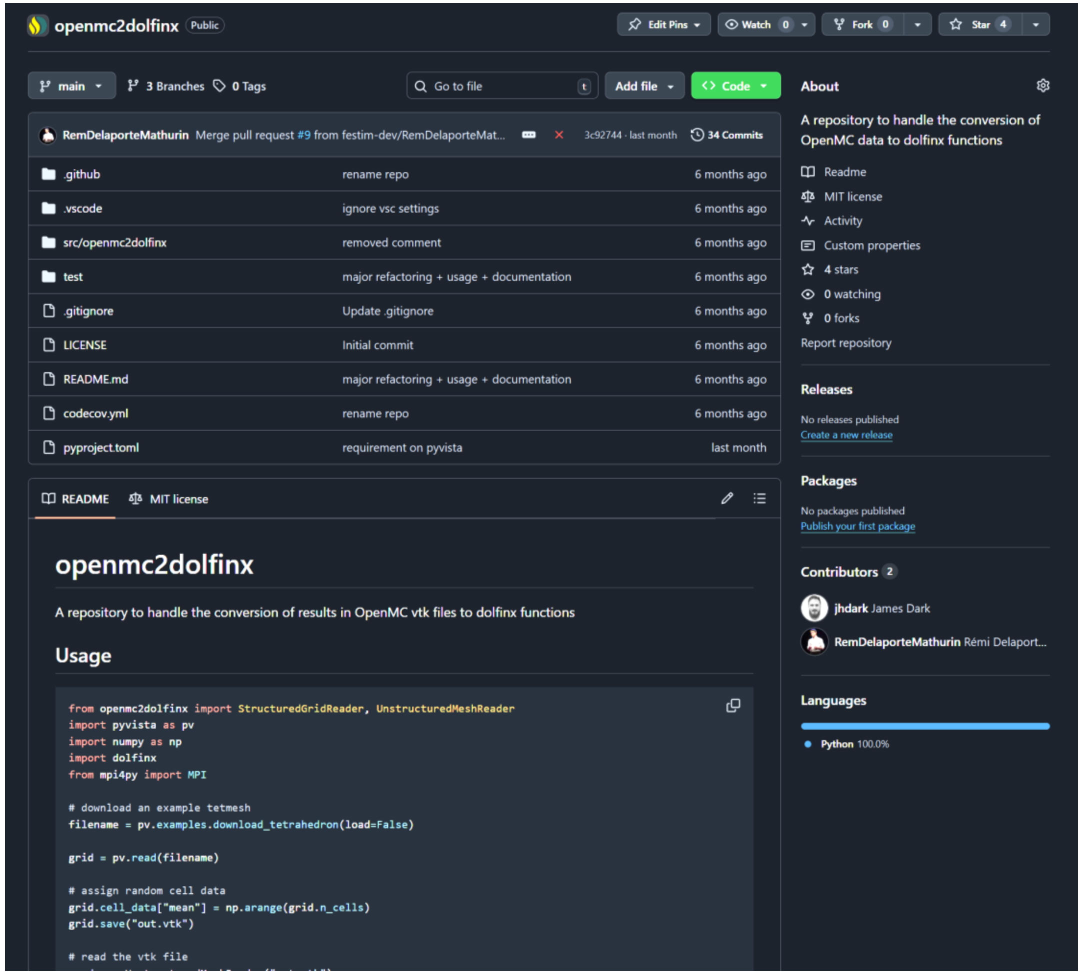


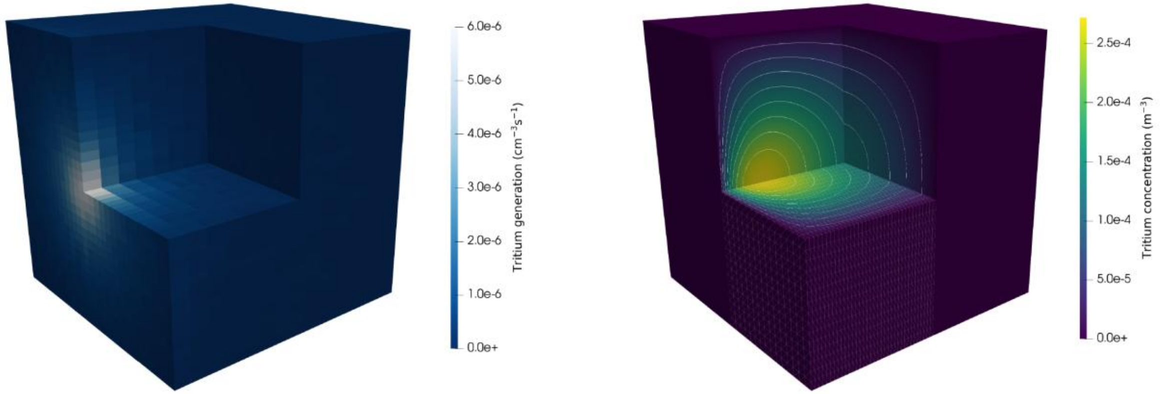
(c) Species concentration without advection



(d) Species concentration with advection

openmc2dolfinx



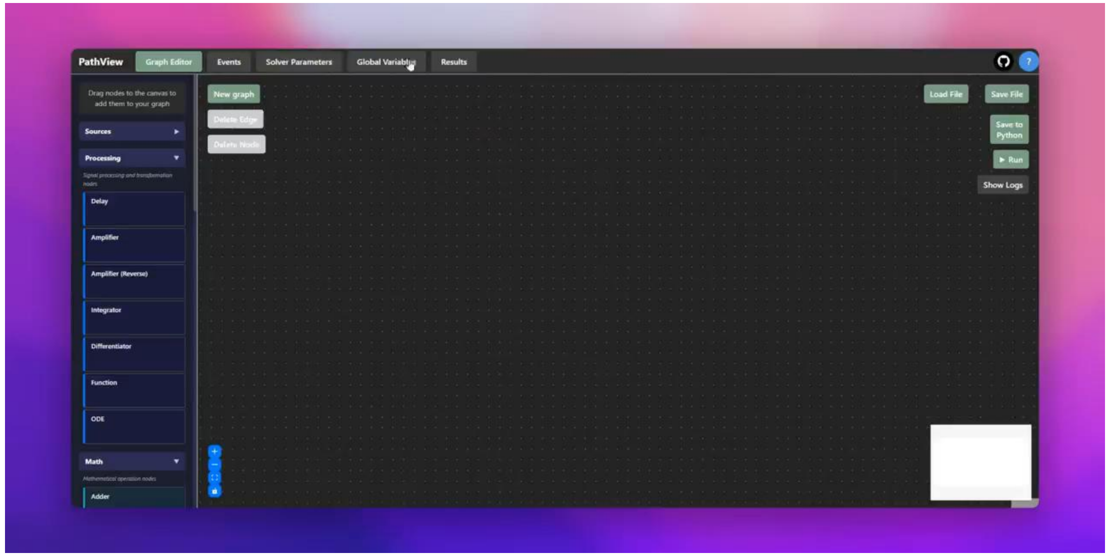


(a) Tritium generation field from OpenMC

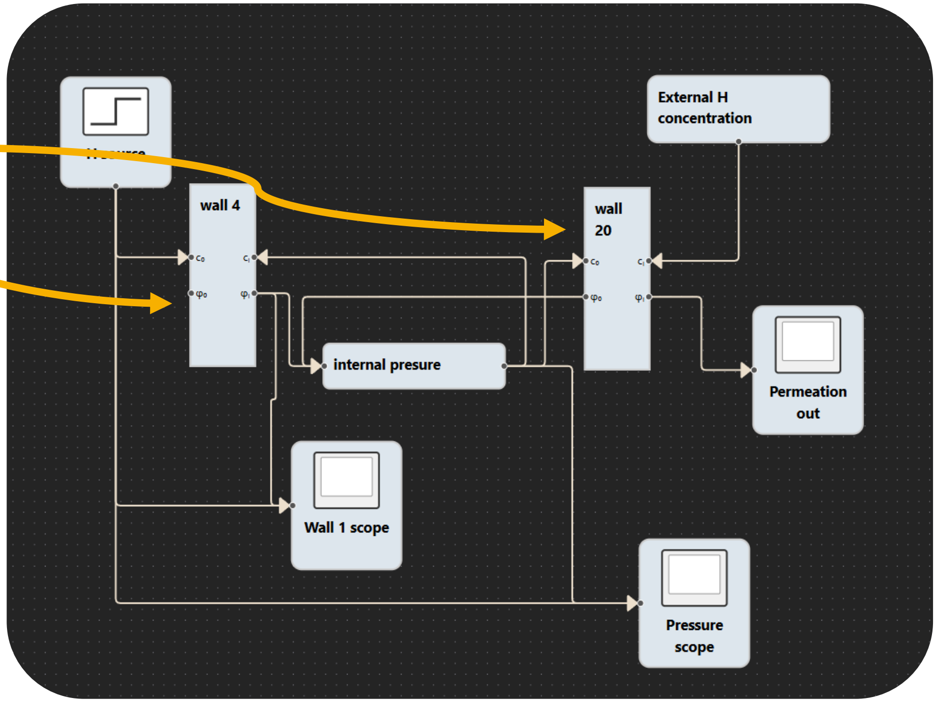
(b) Steady-state tritium concentration from FESTIM

PathView: a new tool for system modelling

- 100% open-source
- Based on PathSim
- Results compared to Matlab Simulink
- Can integrate external tools (eg. FESTIM, ML models/surrogates, …)



Embedded FESTIM simulations!



PathView
github.com/festim-dev/pathview