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FESTIM, a modelling code for hydrogen transport in materials for nuclear fusion applications

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25 March 2021

The principle of nuclear fusion is to fuse two hydrogen nuclei to form a helium nucleus and a neutron, releasing incredible amounts of energy in the process. To achieve these fusion reactions, extremely high temperatures are required: more than 10 times the temperature of the Sun's core. The very hot fuel in the plasma is magnetically confined within a chamber called a tokamak. Eventually, hydrogen ions will hit the reactor walls and penetrate in the materials.

In order to simulate hydrogen transport in complex components (multi-material, multidimensional geometries...), a finite element modelling code relying on FEniCS called FESTIM has been developed [2]. FESTIM solves a set of transient Macroscopic Rate Equations (MRE) which accounts for the diffusion (based on Fick's law) and trapping/detrapping of hydrogen isotopes in materials (based on McNabb and Foster's equations [4]) coupled to transient heat transfer.

This talk showcases the use of FESTIM and FEniCS to model key tokamak components such as actively cooled plasma facing components and how results crucial for the International Thermonuclear Experimental Reactor (ITER) [3] operations are extracted from it [1]. The code was verified using the method of manufactured solutions and validated against experimental results. FESTIM was also benchmarked with other codes from the fusion community and with the commercial simulation suite Abaqus.

This talk was awarded a prize: Best talk by a PhD student or undergraduate.

References

[1] Rémi Delaporte-Mathurin, Etienne Hodille, Jonathan Mougenot, Gregory De Temmerman, Yann Charles, and Christian Grisolia. "Parametric study of hydrogenic inventory in the ITER divertor based on machine learning". In: *Scientific Reports* 10.1:17798 (2020). DOI: 10.1038/s41598-020-74844-w.

[2] Rémi Delaporte-Mathurin, Etienne A. Hodille, Jonathan Mougenot, Yann Charles, and Christian Grisolia. "Finite element analysis of hydrogen retention in ITER plasma facing components using FESTIM". 2019.

[3] "ITER website". http://www.iter.org.

[4] A. McNabb and P. K. Foster. "A new analysis of the diffusion of hydrogen in iron and ferritic steels". In: *Transactions of the Metallurgical Society of AIME* 227 (1963), 618–627.

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FESTIM, a modelling code for hydrogen transport in materials for nuclear fusion applications

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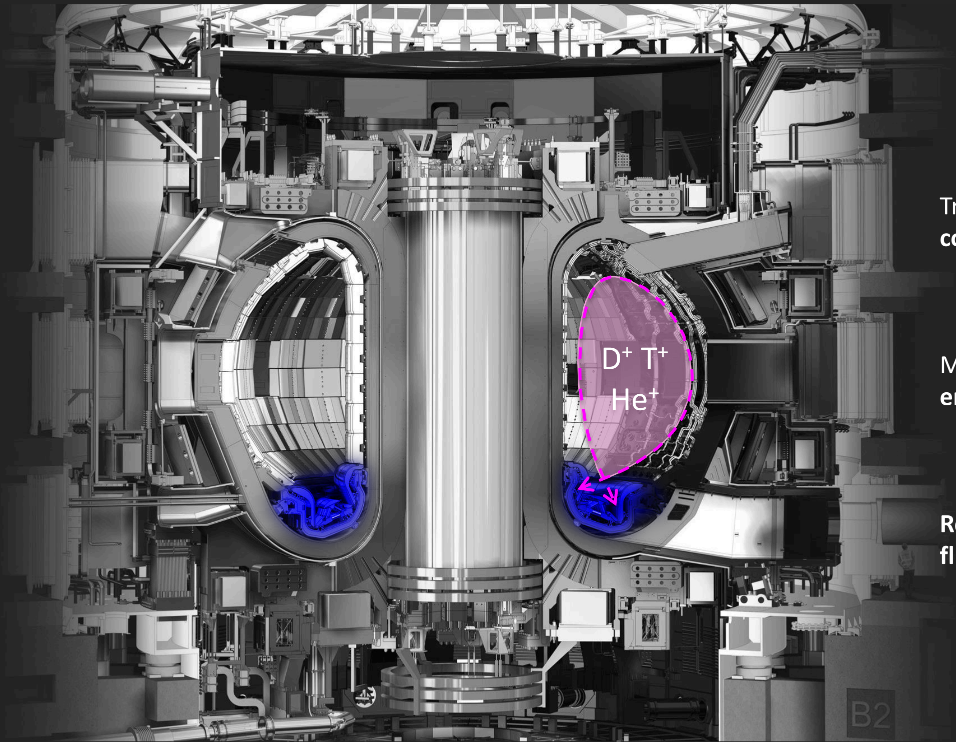


Tritium
contamination

Material
embrittlement

Recycling
fluxes

Images: ITER Organization

$$\partial_t c_\mathrm{m} = \nabla(D(T) \cdot \nabla c_\mathrm{m}) - \sum_i \partial_t c_{\mathrm{t},i} \quad \text{on } \Omega$$

$$\partial_t c_{\mathrm{t},i} = k(T) \cdot c_\mathrm{m}\left(n_i - c_{\mathrm{t},i}\right) - p(T) \cdot c_{\mathrm{t},i} \quad \text{on } \Omega$$

Hydrogen transport
McNabb & Foster - Trans. Metall. Soc. (1963)

$$\frac{c_\mathrm{m}^-}{S(T)^-} = \frac{c_\mathrm{m}^+}{S(T)^+} \quad \text{on } \Omega_i \cap \Omega_j$$

Conservation of chemical potential at interfaces

$$\rho C_p \, \partial_t T = \nabla(\lambda \cdot \nabla T) + Q \quad \text{on } \Omega$$

Energy equation

- $c_\mathrm{m}, c_{\mathrm{t},i}, T$ H concentrations and temperature
- i corresponds to a type of sink

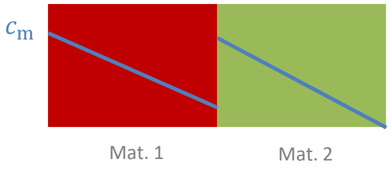
FESTIM

- Finite Element Simulation of Tritium In Materials
- Based on FEniCS
- 1/2/3D
- Multi-materials

For more info:

Delaporte-Mathurin *et al*, NME (2019)

$$\frac{c_\mathrm{m}^-}{S^-} = \frac{c_\mathrm{m}^+}{S^+} \quad \text{at interfaces}$$



- Modelling discontinuities in FEniCS

$$\partial_t c_\mathrm{m} = \nabla(D \cdot \nabla c_\mathrm{m}) - \sum_i \partial_t c_{\mathrm{t},i} \quad \text{on } \Omega$$

$$\theta = c_\mathrm{m}/S$$

1. **Solve** : $\partial_t(\theta S) = \nabla(D \cdot \nabla(\theta S)) - \sum_i \partial_t c_{\mathrm{t},i} \quad \text{on } \Omega$
2. **Post-processing**:

   $c_\mathrm{m} = \theta \cdot S$

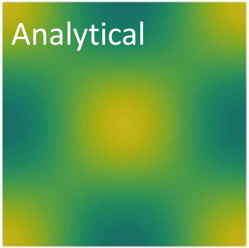
   project on DG1 space

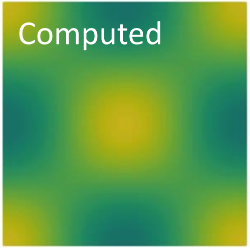
```
V_DG1 = FunctionSpace(mesh, ‘DG’, 1)
c_m = project(theta*S, V_DG1)
```

Delaporte-Mathurin *et al,* Nucl. Fusion (2021)

Verification using MMS

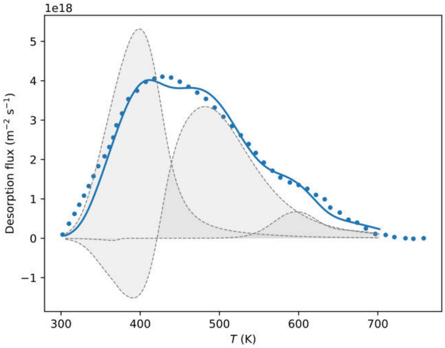
- $c_{\mathrm{m,D}} = 1 + \cos(2\pi x)\cos(2\pi y) + \cos(2\pi t)$
- $T = 500 + 30\cos(2\pi x)$
- Multi-material





Experimental validation

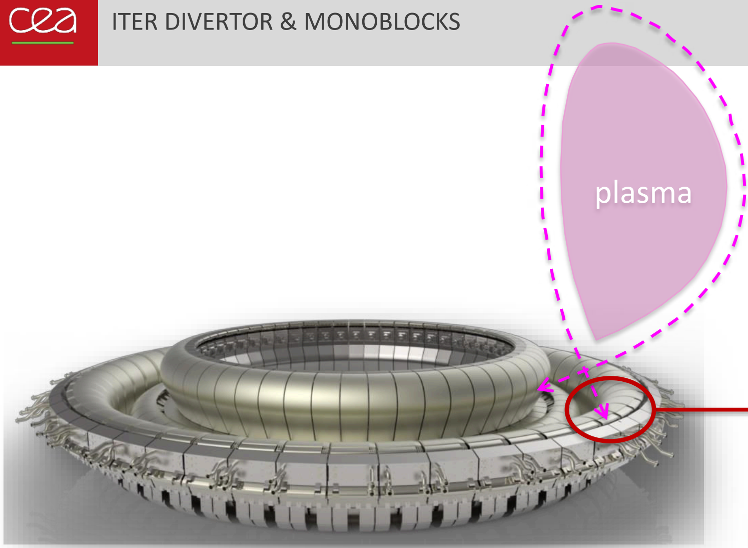
- Thermo-desorption experiments
- Parametric optimisation

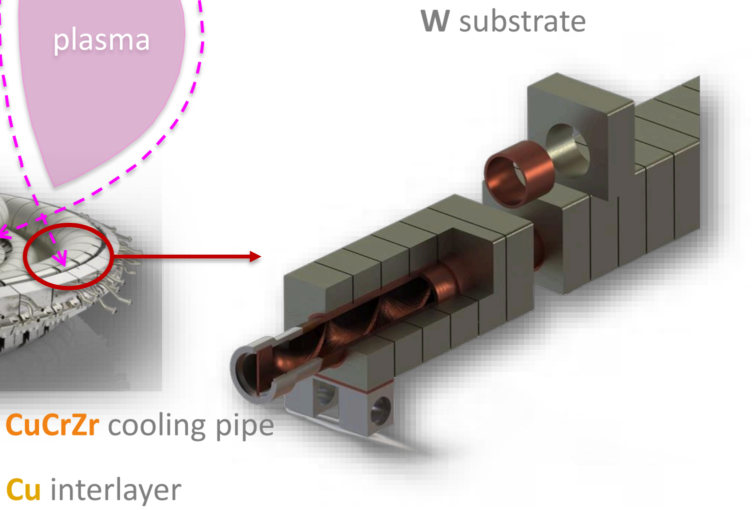


Delaporte-Mathurin *et al,* NME (2021)

Application:

Tokamak components

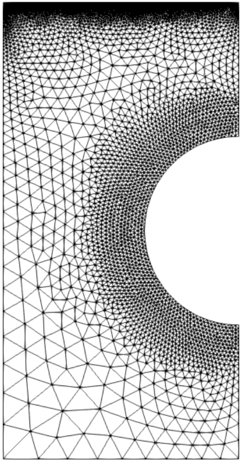




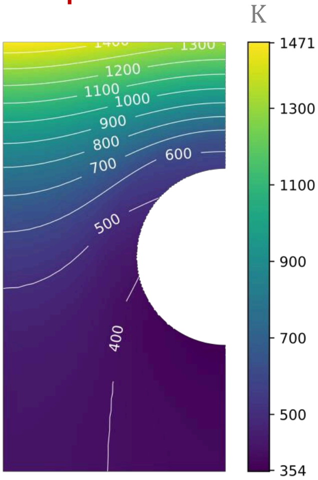
How much hydrogen
is retained ?

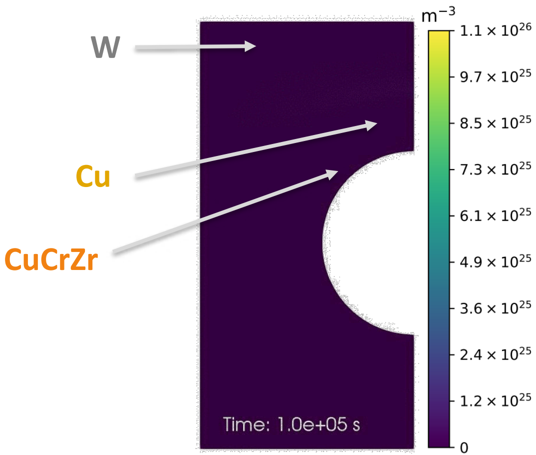
Images: ITER Organization

- Meshed with **SALOME** (open-source)
- Converted from .med to .xdmf with **meshio** [1]
- High refinement:
  - on the top surface
  - at interfaces
- Planned: using Adaptive Mesh Refinement



[1] Meshio: 10.5281/zenodo.4590119

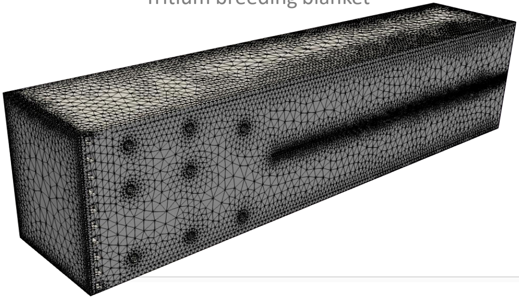


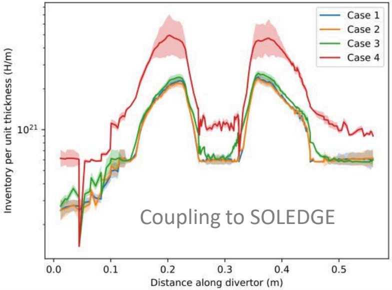


- Total inventory of H : $\int (c_\mathrm{m} + c_t)\, dx$
- Coolant contamination : $\int D(T) \nabla c_\mathrm{m} \cdot \boldsymbol{n}\, dS$

- Applications to more complex tokamak components
- Coupling with other physics
  - CFD
  - MHD,
  - co-deposition models
  - He transport…
- Coupling with external plasma codes

Tritium breeding blanket





Thank you for your attention

Plots were made with Matplotlib and Paraview

- FESTIM is a FEniCS-based simulation interface
- Hydrogen transport (including diffusion and trapping) is modelled and coupled to heat transfer.
- FESTIM applications:
  - Simulating fusion reactors components
  - Identifying materials properties
- Perspectives:
  - Applications to more complex tokamak components (tritium breeding blankets)
  - Coupling with other physics (CFD, MHD, co-deposition models, He transport…)
  - Coupling with external plasma codes (SOLEDGE, SOLPS)

```
import FESTIM

parameters = {
    "materials": [
        {
          "E_D": 0.1,
          "D_0": 1,
          "id": 1
          }
      ],
    "traps": [],
    "mesh_parameters": {
            "initial_number_of_cells": 200,
            "size": 1,
            "refinements": [
            ],
        },
    "boundary_conditions": [
          ],
    "temperature": {
           "type": "expression",
           "value": 300
        },
    "solving_parameters": {
        "final_time": 100,
        "initial_stepsize": 0.1,
        "newton_solver": {
            "absolute_tolerance": 1e-10,
            "relative_tolerance": 1e-9,
            "maximum_iterations": 50,
          }
        },
}

output = FESTIM.run(parameters)
```

```python
class UserCoeff(UserExpression):
    def __init__(self, mesh, vm, T, **kwargs):
        super().__init__(kwargs)
        self._mesh = mesh
        self._vm = vm  # MeshFunction for volume markers
        self._T = T

    def eval_cell(self, value, x, ufc_cell):
        cell = Cell(self._mesh, ufc_cell.index)
        subdomain_id = self._vm[cell]
        if subdomain_id == 1:
            value[0] = self._T(x)
        else:
            value[0] = 2

    def value_shape(self):
        return ()

S = UserCoeff(mesh, vm, T)

V_DG1 = FunctionSpace(mesh, ‘DG’, 1)
c_m = project(theta*S, V_DG1)
```