Upgrading FESTIM for High-Performance Computing with FEniCSx: Mixed Domain Formulation and Enhanced Parallel Scaling

R. Delaporte-Mathurin[1], S. Meschini[1], J.S. Dokken[2], J. Dark[3]

[1] *Plasma Science and Fusion Center, MIT, USA*

[2] *Department of Numerical Analysis and Scientific Computing, Simula Research Laboratory, Norway*

[3] *IRFM, CEA, France*

[4] *LSPM, CNRS, France*

FESTIM (Finite Element Simulation of Tritium In Materials) is an open-source tool designed for simulating hydrogen transport in materials. Since 2019, FESTIM has been extensively used to model tritium transport in fusion relevant components (plasma facing materials, breeding blankets, tritium extraction systems...). While the current version (1.3) is mathematically robust, its performance on high-performance computing (HPC) architectures is limited, particularly in multi-material simulations. This arises from the scaling limitations of some of the post-processing steps in FESTIM necessary due to limitation in the underlying FEniCS finite element engine.

To address these challenges, FESTIM is undergoing a significant upgrade to FEniCSx. This transition introduces the mixed dimensional framework that allows us to directly enforces interface conditions between materials within the governing equations, eliminating the need for post-processing steps. This formulation was not available in the framework initially proposed in legacy-FEniCS. Benchmarks comparing the legacy and upgraded versions of FESTIM show that the new implementation scales much more efficiently in parallel. In a 3D multi-material benchmark, while FESTIM 1.3 saw a fivefold increase in execution time from 1 to 4 processors, the FEniCSx-based implementation reduced execution time by half, with further optimisations ongoing.

Additionally, the new version resolves inefficiencies in modelling material-specific traps. In previous versions, traps had to be defined across entire geometries, even when they only applied to certain subdomains, leading to wasted computational resources. The new implementation addresses this by localising traps to relevant subdomains.

Looking ahead, FESTIM 2.0 will incorporate mixed topology meshes, multi-species (multi-isotope) capabilities, and support for external physics solvers like OpenFOAM and OpenMC, making it a more versatile tool for hydrogen transport simulations.