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Code coupling library for Multiphysics CFD and Solid Stress software for HPC Verification

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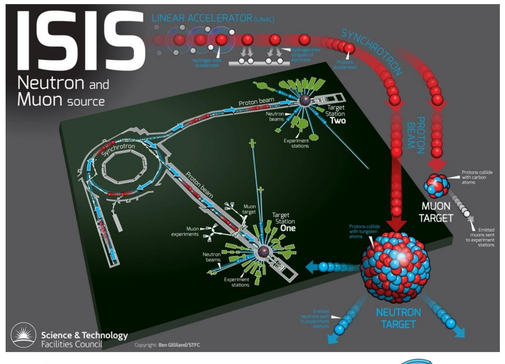
This project couples programs that model thermoelastic effects with computational fluid dynamics for engineering the neutron and muon spallation source target, TS2 at ISIS.

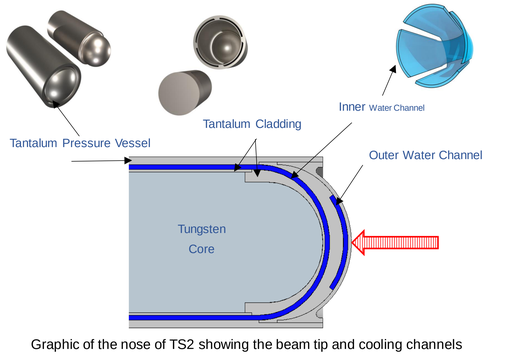
The ultimate aim is to develop a Multiphysics code coupling library that will be useable in a container, meaning it can be run in a diverse range of supercomputing environments. The two open-source software packages which are the focus; Code_Saturne for CFD and FEniCSx, a finite element solver, are both being developed for parallel computing that can be run on platforms from laptops to HPC's.

The project has an emphasis on considerations for parallel computing, how it can be used for productive HPC and the ease of use of the new open source software library.

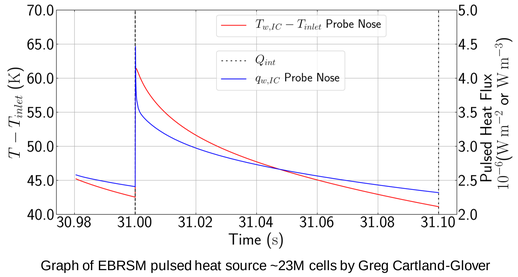


At ISIS, beams of protons are accelerated up to 80% the speed of light and ejected at target station 2 (TS2). The resulting neutron scattering allows for material properties to be measured for applications in medicine and engineering.

TS2 is made from Tungsten with a Tantalum casing,and has two water cooling channels. As the proton beam meets the nose, it experiences a periodic temperature change, causing stress throughout the target that limits its lifetime.
Improvements would hope to save resources, reduce downtime and prevent radioactive waste.

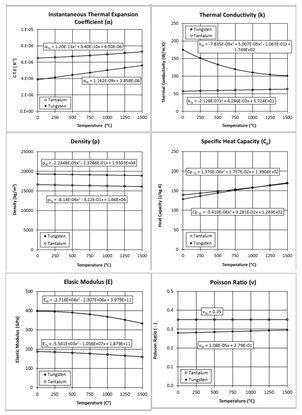


Graphic of the nose of TS2 showing the beam tip and cooling channels

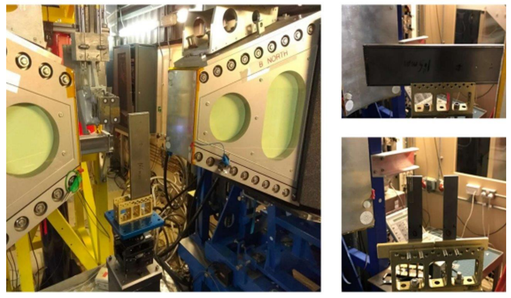


Graph of EBRSM pulsed heat source ~23M cells by Greg Cartland-Glover

There are many contributions to take into consideration for the stress, as the two metals have different material properties meaning there is tensile stress in the cladding as it contracts more than the core as it cools leaving residual stresses throughout.

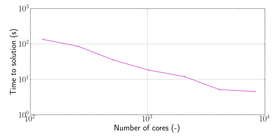


Models such as this are created using a variational formula of the heat equation for a body of dual materials, and equations governing small elastic deformations of a body. This involves writing a python script using the FEniCSx library of PDE solvers over a GMSH mesh using the Finite Element Method. There is a model in development for a fully coupled thermoelastic evolution problem, to model thermal expansion and stresses in a two-layer metal plate. For a fully coupled time-dependent thermal elastic simulation, mixed function space with displacement and temperature is essential, which has been implemented in the main branch of FEniCSx.



The ENGIN-X experiments that provide the test data on the dual material plate

Challenges of the project
- Multiphysics Problem
- Stress concentrations from geometry
- Concurrent simulations
- Mesh communication
- Code coupling
- Current models
- Sensor data



Parallel Scale-up on Archer 2 with ~100M cells

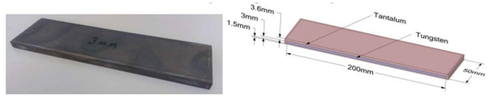
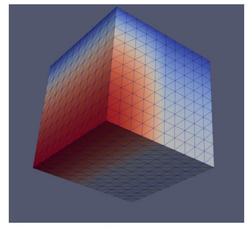
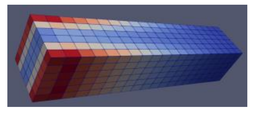


Photo and schematic of the test piece used for ENGIN-X experiemental test data

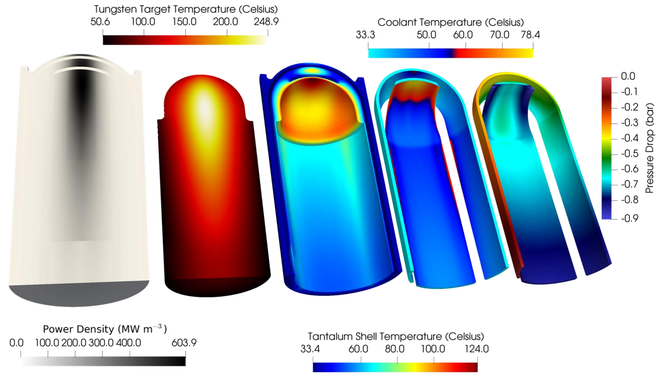


Visualization in Paraview of a dual material mesh using Poisson Equation (above) and modelling Von Mises stress (below) written using FEniCSx PDE solver



Current options for coupled code models are limited by cost, licensing and resolution, and don't hold capacity for HPC. Code Saturne is a highly parallelisable software for computational fluid dynamics, which does not have a licensing limitation.

The next steps will be to set the material properties for a tantalum clad tungsten plate for validation against ENGIN-X measurements. When the code is verified, this can be applied to the geometry of the target, before being coupled to conjugate heat transfer calculations.
The final step in this will be to use the target model of thermal stresses to couple with RANS calculations of the target or the cooling channels of the target.



CHT with EBRSM turbulence ~23M cells (16M solid+7M fluid)

Modelling Pulsed Heat Source CHT of TS2
- We will model fluid flow in the channels with Code_Saturne and exchange surface temperature and its gradient with solid model of TS2 in FEniCSx to which the pulsed heat source is applied
- Have run cases using ~215 million cells on Archer 2 using 32 nodes and 16 and 32 nodes of Scarf using 23 million cells for conjugate heat transfer results
- Conjugate heat transfer with pulsed heat source
- Temperature using ~ 23 million cells (16M solid + 7M fluid)
- Use pulsed EBRSM model and exchange volume or surface temperature data with solid model of TS2 in FEniCSx

This project will build a library that will allow us to couple key engineering considerations between intricate finite element mesh's running on separate programs. This will be applied to a model of the ISIS TS2 and compared to current models and sensor data from ISIS for verification. The result is a suite of programs and libraries that can model thermal elastics coupled to conjugate heat transfer. It will be useable as a high-resolution, open source, HPC Library for Multiphysics code coupling. Importantly, it has the potential to provide accurate supercomputer benchmarking of lower resolution, computationally less intensive, CFD and Solid Stress models.

archer2 SCARF ParaView FEniCS project Gmsh code_saturne