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ABSTRACT

We present new two applications, `AURORA` and `Achlys`, developed using the `MOOSE` framework for finite element analysis, intended to facilitate engineering analysis for fusion reactors. Respectively these couple neutronics and tritium transport to native `MOOSE` physics modules including heat conduction and tensor mechanics. We outline steps taken to perform verification of software and validation of physics models. We provide a proof-of-concept application to a breeder blanket model, drawing some qualitative conclusions. Finally, we consider future directions for further in-depth analysis and development.

KEYWORDS: Multiphysics, Fusion, Breeder Blanket, Neutronics, Tritium transport

1. INTRODUCTION

Progress towards the development of a commercially viable, magnetic confinement fusion reactor is rapidly accelerating. In this domain, there is a growing need for high fidelity engineering design and analysis software tools capable of simulating the immensely complex multiphysics and multiscale environment of a tokamak reactor. Our aim in addressing this need is to develop a suite of tools each tailored towards a specific area of physics relevant to fusion, and capable of independent execution, yet intended to operate within a larger integrated package.

There are considerable overlaps between the physics simulation concerns of nuclear fusion with that of nuclear fission; examples include the need for modelling of coupled neutronics, structural mechanics, thermodynamics and fluids. Given the need for both rapid development, verification and validation in what will be a regulated industry, it is highly desirable to build upon the wealth of existing knowledge gained from a long history development for fission reactors. Provided any implementation of common tools entails sufficient levels of generality, it is likely that there should arise some natural symbiosis between the two communities. In practice, we leverage a number of existing software packages already proven in fission applications.

As a starting point, we have chosen to develop our code using the `MOOSE` (Multiphysics Object-Oriented Simulation Environment) framework [1–3]. This design choice was influenced by a number of factors [4]. First, as with small modular fission reactors, the detailed modelling of a tokamak is projected to be an exascale endeavour [5] so parallel performance is paramount; `MOOSE` has been shown to scale to many thousands of cores [1]. Second, a requirement to be open source; this stems from a need for flexibility in implementing new features, incorporating additional dependencies, and portability between architectures. Finally, `MOOSE`'s modularity and ability to run hierarchical and recursively organised sub-applications (via the `MultiApp` class) makes it highly conducive to the development and coupling of multiscale, multiphysics applications.

Notwithstanding those similarities between fusion and fission to which we have already alluded, simulation for fusion also exhibits some additional unique challenges. The presence of huge magnetic fields will exert immense forces on structural components, yielding additional sources of deformation. For example, the ITER toroidal magnets may generate field values of order 12 T leading to circumferential tension of order 100 MN [6]. Plasma-facing components will be subject to extreme heat loads ($\gtrsim 0.5 MW m^{-2}$) that must be cooled over small spatial distances resulting in enormous temperature gradients. The necessity to sustainably fuel the fusion reactions requires breeding of tritium. We seek to address these challenges and more as we develop a suite of tools to cater for fusion reactor simulation.

Since a high-fidelity multiphysics modelling of an entire tokamak is still some way off, both in terms of the maturity of software and availability of exascale computing, for the medium term we intend to first target simulation of some critical components. Such components must act as a microcosm for the wider tokamak reactor environment, featuring the integration of all essential physics areas. The breeder blanket, responsible for capturing neutrons and converting their energy into heat, while simultaneously breeding tritium, represents one such targeted critical component.

In a first step towards this goal, we present two tools recently developed using the `MOOSE` framework, and apply these to a simplified blanket geometry as a proof-of-concept. The first is `AURORA`, designed to couple neutronics from `OpenMC` [7,8] with `MOOSE`'s native heat conduction and mechanics modules. The second is `Achlys`, designed to incorporate tritium transport. Both feature among a growing suite of fully open-source tools, which may be found at https://github.com/aurora-multiphysics.

The paper is organised as follows. In section 2 we describe `AURORA`, focusing in particular on the mechanisms of coupling. In section 3 we describe `Achlys`, including details both of mathematical model, verification, and validation against another code, `FESTIM` [9]. In section 4 we present the results of coupling `AURORA` and `Achlys` for the simplified blanket model. Finally we present our conclusions and outlook in section 5.

2. COUPLED NEUTRONICS AND THERMOMECHANICS WITH AURORA

2.1. Implementation

`AURORA`* is an application developed within the `MOOSE` framework to couple the neutron transport from `OpenMC` with heat conduction and thermal expansion. Underpinning this coupling is the expectation of large temperature gradients and local density changes from thermal expansion induced by neutron heating. Since nuclear cross sections themselves depend on these quantities, the raison d'être of `AURORA` is to feed these transient fields as computed by `MOOSE` back into the `OpenMC` calculation. The method through which this is implemented will be examined below.

To enable neutron transport on arbitrary geometries, `OpenMC` employs `DAGMC` [10] to perform particle tracking through logical volumes enclosed by faceted surfaces. Tallies for quantities of interest such as flux and heat may be scored upon an additional unstructured tetrahedral mesh. For our purposes, both surface and volume mesh are represented in memory using the library `MOAB` [11,12], though we note the recent integration of `libMesh` [13] into `OpenMC` which may be employed in future.

In order to obtain `OpenMC` tallies that have a direct correspondence in `MOOSE` it is necessary to have the same underlying geometries in each. In `AURORA` therefore, the `MOAB` encapsulation of the volume† mesh is instantiated in memory directly from that contained in `MOOSE`. Once unstructured mesh tallies are obtained from `OpenMC` these may be directly transferred into `MOOSE` variables for use in transient finite element analysis (FEA). In particular, the heat deposited from neutrons is utilized as a source term for

*The name `AURORA` is an acronym for “A Unified Resource for OpenMC (fusion) Reactor Applications”.

†The initial `DAGMC` surface mesh for the zeroth timestep is currently read from file, though this is a redundant step we intend to eliminate in future.

heat conduction, whereupon the resulting temperature distribution may be solved. Displacements of the mesh arising from thermal expansion may also be solved for simultaneously, and the resulting density field subsequently computed.

Having completed a given MOOSE timestep, it is possible to sort elements of the unstructured mesh according to their binned results for temperature and density. This permits the definition of local regions in which these quantities are deemed to be constant. Applying the so-called skinning operation from MOAB to these grouped elements provides the surfaces and implicit volumes required by DAGMC which may be associated with the appropriate material properties and cross sections within OpenMC. It is now possible to repeat the OpenMC simulation and subsequent procedure for as many timesteps as desired or until some stopping criterion is reached (e.g. steady state or a limiting component temperature is attained).

We contrast our approach with that of another recently developed application, Cardinal [14]. Similarly to AURORA, Cardinal also interfaces OpenMC to MOOSE, with the addition of NekRS [15] for fluids, and BISON [16] for its nuclear fuel modeling capabilities. In its original application to pebble-bed reactors, it was sufficient to create feedback in the form of *average* quantities per pebble. Specifically, OpenMC provides the average heat source per pebble, and is updated with the average temperature; there is no update of material regions in between OpenMC iterations. Volumes are created in OpenMC through its native constructive solid geometry (CSG) methods (i.e. in terms of quadratic surfaces) so do not have a direct counterpart in MOOSE, and thus there is currently no mechanism to update the geometry in response to e.g. deformation.

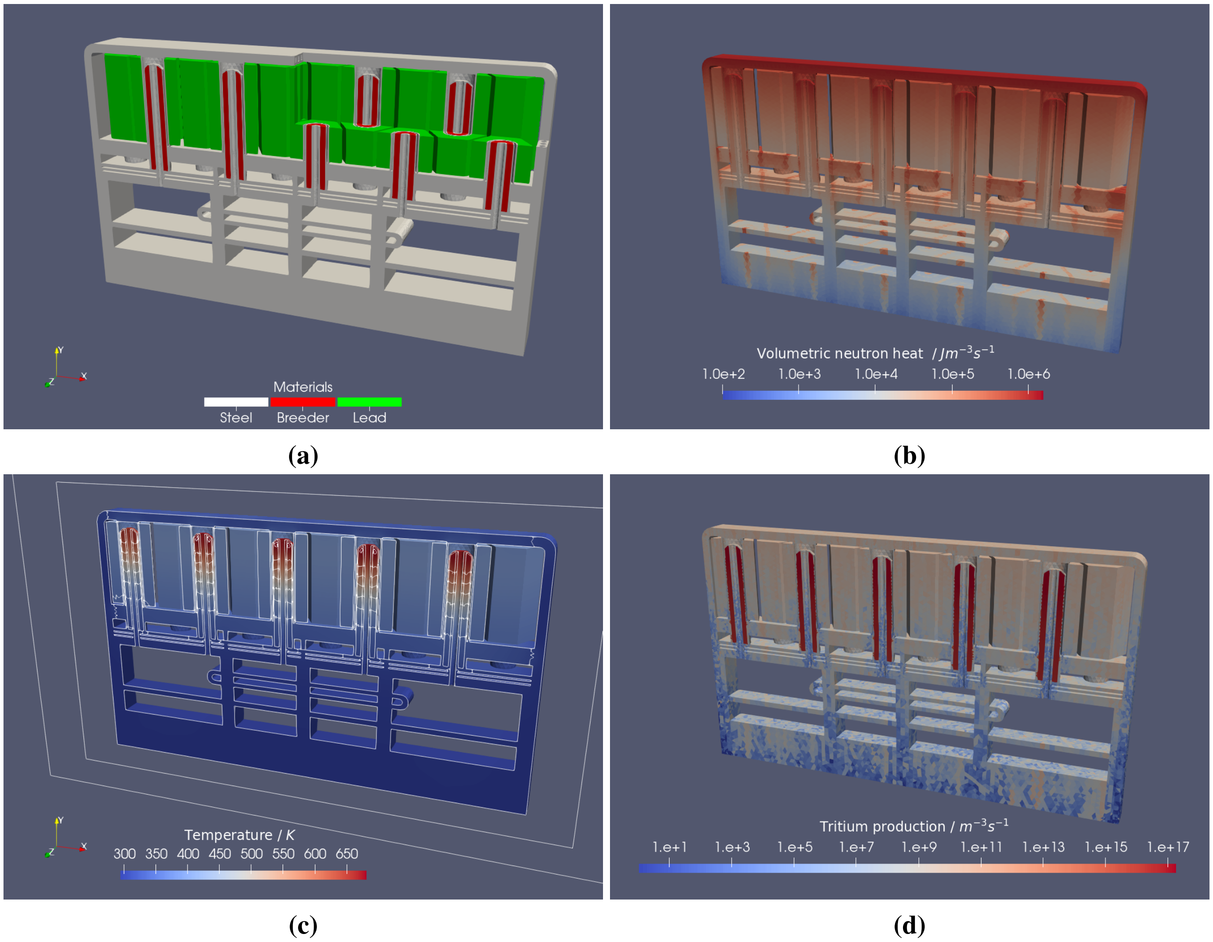
2.2. Preliminary Results

Since OpenMC and MOOSE are already validated independently we do not repeat this step here; may it suffice to note that the coupling interface between these tools has been extensively verified through a suite of unit and integration tests that also comprise our continuous integration. We reserve a validation of the feedback mechanism against experimental data to future study, since such an analysis will require consideration of additional effects such as cooling from fluids and is beyond the scope of the present work. Instead, we here present a selection of results which qualitatively demonstrate the capabilities of AURORA simply as a proof-of-concept.

Our model comprises a section of a DEMO-like Helium Cooled Pebble Bed (HCPB) breeding blanket [17,18], in which tritium breeder pins are surrounded by a neutron-multiplier material in a hexagonal arrangement. In our simplified set-up whose geometry is shown in fig. 1a, we consider only three material designations: for the breeder pin we take Lithium Orthosilicate (Li_4SiO_4); for the neutron-multiplier, lead (Pb); for the remaining support structure, steel. Upon the surfaces interfacing to cooling channels we apply heat flux boundary conditions in lieu of proper fluid modeling. The physical dimensions of the model are $1.4 \times 0.8 \times 0.1 m^3$; the tetrahedral mesh used for finite element analysis has 1.6×10^5 degrees of freedom.

A transient analysis for the model was performed with AURORA across 1000s in timesteps of 30s. The neutron source was taken to be a fixed plane source in the $x - z$ plane at $y = 0.88m$, having a strength of $10^{17} s^{-1}$. In this study, we did not consider displacements of the mesh.

Visualizations of some selected quantities of interest corresponding to the final timestep are shown in fig. 1. The neutron heat flux, which constitutes the heat source that drives an increase in temperature, is shown in fig. 1b. The temperature field, along with contours which define material regions as updated within OpenMC is shown in fig. 1c. Qualitatively we observe that although the entire component is strongly irradiated, the steel support remains at a low temperature as a consequence of cooling and its heat transport properties, whereas in the multiplier and pins the temperature continues to rise. Finally, the concentration of tritium is shown fig. 1d. In line with expectations, tritium is produced primarily in the breeder pins. The production rate falls by around 8 orders of magnitude when transitioning from the breeder into the surrounding materials. For this reason it was challenging to obtain a good statistical convergence in some



(a) (b) (c) (d)

Figure 1: Example of results produced with AURORA for the HCPB breeder blanket model.

elements, in particular those furthest from the source (where the flux was also lowest), where the uncertainty may be as much as 100%. This effect is visible in the granularity in the results in this region. Although these errors could be reduced by increasing the number of particle histories, already 200 batches of 5×10^6 particles were used, requiring 10 MPI tasks and 56 threads per task. Reducing these uncertainties further was beyond the scope of this particular study, and moreover does not impact the conclusions, these being more focused towards a demonstration than on precise analysis.

We conclude this section by noting that even for this relatively simple model, AURORA demonstrably constitutes a platform for a sophisticated analysis of coupled neutronics and thermodynamics. We postpone a more in-depth case study of its usage to future work.

3. TRITIUM TRANSPORT WITH ACHLYS

3.1. Implementation

The Achlys MOOSE application is concerned with the transport of hydrogen isotopes (HI) in different materials and implements a transient diffusion-trapping equation to track HI concentrations, often over whole component lifetimes. This topic is an area of interest in the design of magnetically-confined fusion devices for a number reasons, outlined as follows.

Firstly, the mass of radioactive tritium which accumulates in the plasma-facing components must be understood on the grounds of nuclear safety; for example, the ITER licence limits in-vessel tritium retention to 1kg [19]. The ability to predict precisely how much tritium is trapped in the first wall material (as opposed to permeating into the cooling channels) remains a topic under active investigation [20].

Secondly, the favoured fuel for the current generation of fusion devices is a deuterium-tritium mixture where the tritium must be bred in-situ using lithium-based blankets. In this context, understanding the permeation of hydrogen isotopes through various materials is necessary for the design of the storage and delivery systems of the hydrogen-based fuel cycle. Some attempts have begun in this context to fully characterise and model the HI transport phenomena for DEMO breeder blankets [21].

Finally, elevated hydrogen concentrations within certain materials can lead to degradation of their structural properties, such as hydrogen embrittlement, and the release of gasses such as hydrogen from first-wall materials can interfere with the core plasma properties during operations.

For these reasons, it is desirable to have simulation tools which can track the evolution of HI concentrations through mixed materials and often complex geometries. A number of well-established tools already exist: `FESTIM` [9], `MHIMS` [22], `TMAP` [23], `TESSIM-X` [24]. Notably, `FESTIM` has been used extensively in the most recent ITER studies [20].

The primary motivation for an implementation within `MOOSE` is to utilise anticipated couplings to other physics modules such as `AURORA` (to be explored in section 4), and study the impact on tritium diffusion from precisely-calculated thermo-mechanical loading experienced in metre-scale components and assemblies. However, even as a standalone tool, `Achlys` presents new opportunities: by leveraging `MOOSE`'s proven scalability it will be possible to tackle a new scale of problem not yet attempted in this domain in high fidelity and in three dimensions. Furthermore its open source implementation will facilitate future benchmarking and comparisons to data. `Achlys` adopts exactly the same formulation of underlying equations as `FESTIM` allowing for validation against numerous published results.

Concretely, `Achlys` implements the Foster-McNabb trapping-diffusion equation [25], with coupled heat transport. This model accounts for two phases on HI: (i) mobile, where it can diffuse freely through the material, and (ii) trapped within any number of sites (representing different microstructural features such as lattice vacancies) that immobilise HI atoms. The concentrations of the mobile phase, C_m, and within each trapping site, $C_{t,i}$ are captured by

$$\frac{\partial C_m}{\partial t} = \nabla \cdot (D \nabla C_m) - \sum \frac{\partial C_{t,i}}{\partial t} + S_{ext} \tag{1}$$

and

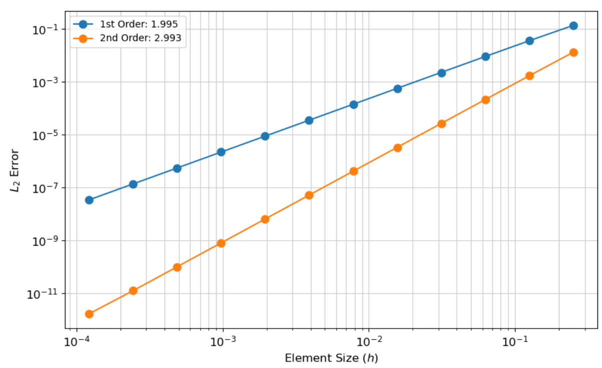
$$\frac{\partial C_{t,i}}{\partial t} = \nu_m C_m (n_i - C_{t,i}) - \nu_i C_{t,i} \tag{2}$$

respectively. Here, D is the diffusivity, S_{ext} is an external source rate, n_i is the concentration of the i^{th} trap type. Transport between the trapped and mobile phases is modelled as temperature-activated reactions: ν_m is the trapping reaction rate and ν_i is the rate of de-trapping from the i^{th} trap.

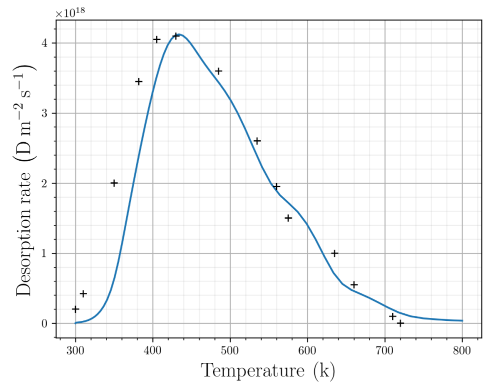
The above model can be captured using existing kernels from the `MOOSE` framework, except for the balance between the trapping and de-trapping reactions, shown on the right hand side of eq. (2), for which a custom kernel has been developed. Coupled heat transfer is also taken into account using the `MOOSE` heat conduction module, as all the transport processes are highly temperature dependent.

3.2. Preliminary Results

An overview of the verification and validation of the `Achlys` code will be presented below, though further details are reserved for future publication. Verification of `Achlys` has been conducted through both



(a) `Achlys` spatial convergence test for first and second order elements using the method of manufactured solutions.



(b) Plot showing a comparison of `Achlys` against data [26] for desorption rates as a function of temperature.

Figure 2: Examples of `Achlys` verification and validation studies.

comparison to analytical solutions and the Method of Manufactured Solutions (MMS). The analytic solution to a one-dimensional diffusion problem with a single trap is described extensively in the literature [27,28]. The comparison of `Achlys` to the exact results for this case is provided as an example in the code documentation. The method follows that described in [9] and good agreement is obtained.

Verification of `Achlys` using the native capability for MMS in `MOOSE` showed the expected convergence behaviour for both first- and second-order schemes for both spatial and temporal convergence cases. An example for the spatial test is shown in fig. 2a where the $L2$ error as a function of element size h should decrease as h^{N+1}, with N the order of the element. The calculated $N+1$ value for each line is shown in the legend of this plot, both of which approach the ideal values and indicate the test has passed.

Validation was performed through comparisons to published experiments and simulations, including tritium accumulation in the ITER divertor as well as deuterium implantation and desorption in thin tungsten foils [26]. In all cases, `Achlys` was found to successfully reproduce `FESTIM` results [9,20].

An example validation case is shown in fig. 2b which aims to model the experimental set-up for measuring thermal desorption spectra from [26]. In this experiment a thin tungsten foil is initially loaded with a beam of deuterium ions. After the beam is switched off, the rate of release of deuterium gas is measured as the material sample is heated at a constant rate of $8\ \mathrm{K\,s^{-1}}$. The simulation tracks the evolving spatial distribution of deuterium in the different mobile and trapped phases, both during implantation and throughout the subsequent temperature ramp. The result in fig. 2b shows the simulated outward flux through the external surfaces of the tungsten foil as it is heated. The `Achlys` simulation here uses exactly the same input parameters as were used by `FESTIM` in [9]. This result is qualitatively very similar to that produced with `FESTIM` , though the `FESTIM` data was not available for a direct comparison.

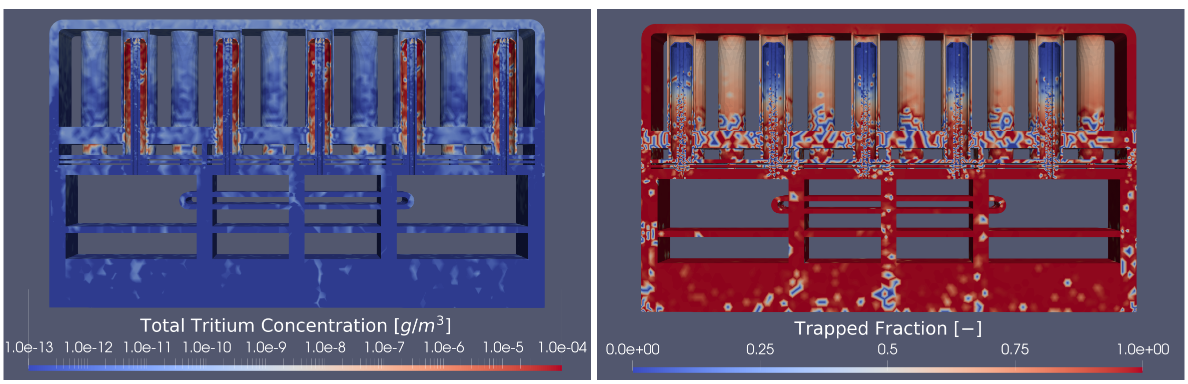
4. COUPLED ANALYSIS OF THE HCPB BREEDER BLANKET

Having demonstrated the independent capabilities of `AURORA` and `Achlys` in sections 2 and 3 respectively, we now consider the impact of coupling these tools. Although there is no direct coupling of these tools in memory at present, we see no conceptual barrier to implementing one in future. For this indicative study however, results taken from `AURORA` are written to file and subsequently read into `Achlys`.

As the model for our study we take the HCPB breeder blanket that was already described in section 2.2. Two time-dependent variables taken from AURORA are of consequence to Achlys: the production rate of tritium, and the temperature distribution, upon which the rates of trapping and desorption are highly dependent. Taking these fields as input, Achlys can provide insight into the resulting distribution of tritium retained in the steel structure (and whether it resides in the trapped or mobile phase) and the rate at which this leaks into the coolant channels.

Figure 3a shows the total tritium concentration accumulated by the end of the timestep corresponding to 1000s. A very high concentration region can be seen in the steel cladding directly supporting the breeder material. High production rates and temperatures in the breeder drive rapid diffusion into the surrounding steel here. Some tritium is also produced directly within the steel structure as a result of the neutron bombardment which can be seen particularly on the top surface. In future studies this could be tracked for the whole lifetime of the component as the time scales for the build-up and diffusion of tritium in steel is much longer than the time for the blanket module to reach thermal equilibrium under neutron loading. The granularity in these results relates to the challenges of statistical convergence where the production rates are very low, as discussed previously in section 2 for the AURORA simulation.

Figure 3b shows the fraction of existing tritium in the trapped phase. It can be seen here that the relatively low temperatures simulated highly favour the trapped phase. This situation is a current concern in blanket simulations for DEMO [21] where tritium trapped in structural steels cannot be released as the high temperatures required would compromise the mechanical properties required of these components. Understanding sink-terms like this is important for predicting the effective rate at which tritium gas can be produced and extracted from different breeder blanket designs.



(a) Tritium concentration in steel structure after 1000s of neutron irradiation.

(b) Fraction of existing tritium which resides in the trapped phase.

Figure 3: Example Achlys results for tritium transport coupled to AURORA output.

5. CONCLUSION AND OUTLOOK

In this paper we presented two recently-developed open source MOOSE applications, AURORA and Achlys, which are available at https://github.com/aurora-multiphysics. These have been designed to provide high-fidelity multiphysics and multiscale engineering simulation to support the effort to design a commercially viable fusion reactor. Building upon existing open source software developed with fission applications in mind, these tools address new challenges that arise in fusion environments. In anticipation of large thermal gradients, AURORA couples the impact of heat conduction and thermal expansion into neutron transport provided by OpenMC. To assess the impact of the wider environment upon the ability to breed tritium, and likewise the impact of tritium build-up within an entire component, Achlys implements transport of hydrogen isotopes.

To provide a proof-of-concept demonstration, we performed a transient simulation for a section of a HCPB breeder blanket. Although an in-depth analysis is postponed for future work we can nevertheless make some simplistic conclusions. The breeder material steadily increases to high temperatures as neutrons deposit heat, while the surrounding materials remain relatively cool. Primarily tritium is produced within the breeder material as should be expected, but as a consequence of some initial concentrations, diffusion of the mobile phase driven by high temperature, and finally trapping, it is likely that some proportion will likely remain in the steel structure when considered over much longer time scales.

These qualitative observations promote a number of questions which the combination of `AURORA` and `Achlys` will be uniquely placed to address. We can examine to what levels tritium accumulates in a given component over its entire lifetime, how this is impacted by given levels of neutron irradiation, temperature and material deformation, and whether this adheres to safe limits. We can assess the long term impact of damage from hydrogen embrittlement upon structural integrity. We can investigate to what extent leakage of tritium into the structure impact the final levels that can be usefully extracted for fuel. These questions and more provide a wealth of avenues for future study, and provide ample justification for our implementations.

The initial couplings presented here represent only a first step towards a much more ambitious multiphysics vision for fusion simulation. To fully capture a component such as a blanket will require additional couplings to electromagnetism, fluid dynamics, (or possibly magnetohydrodynamics in the case of liquid metal blankets), and material damage. To reach this goal will involve a similar pattern as presented here: implement and validate each natural physics area independently, then systematically introduce couplings and investigate their impact in increasingly complex cases. From a software perspective, this strategy has been much enabled by use of the `MOOSE` framework.

Going forwards, it will be necessary to identify high quality validation cases that demonstrate the accuracy of the multiphysics couplings. This could include new state-of-the-art experimental facilities at UKAEA such as HIVE ("Heating by Induction to Verify Extremes") for thermofluid and thermo-mechanical verification of high heat-flux components [29] and CHIMERA ("Combined Heating and Magnetic Research Apparatus") for metre-scale in-vessel component studies [30].

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