HORIZON-EUROHPC-JU-2021-COE-01

EXCELLERAT P2

The European Centre of Excellence for Engineering Applications

Project Number: 101092621

Updated Report on the L2G/OpenFoam/Raysect Application Use Case

The EXCELLERAT P2 project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101092621. The JU receives support from the European Union's Horizon Europe research and innovation programme and Germany, Italy, Slovenia, Spain, Sweden and France.

Work Package:	2	Updated Report on the L2G/OpenFoam/Raysect Application Use Case	
Author(s):	Matic Brank		University of Ljubljana
Approved by	Executive Centre Management		12.12.2025
Reviewer	Ansgar Niemöller		RWTH
Reviewer	Simone Bna'		CINECA
Dissemination Level	PU - Public		

Date	Author	Comments	Version	Status
2025-04-29	Matic Brank	Initial draft	V0.1	Draft
2025-05-07	Ansgar Niemöller	First revision	V0.2	Revision
2025-05-09	Simone Bna'	First revision	V0.3	Revision
2025-05-16	Matic Brank	Second draft	V0.4	Draft
2025-05-19	Ansgar Niemöller	Second revision	V0.5	Revision
2025-05-26	Matic Brank	Final version	V1.0	Final
2025-12-10	Matic Brank	Revised version based on JU reviewers' comments	V2.0	Final

List of abbreviations

UL	University of Ljubljana
ITER	International Thermonuclear Experimental Reactor
CEA	Centre of Atomic Energy, Cadarache
F4E	Fusion for Energy
FVM	Finite Volume Method
IR	Infra-red

Executive Summary

This document summarises the progress made since M12 in the FA-1 use case (UC) by University of Ljubljana. The objective and the development of the use case workflow with detailed description is presented. First, an introduction is made which explains the purpose and extent of the use case with respect to research in magnetically confined nuclear fusion. Then the objective of the case is explained and its aim with respect to the EXCELLERAT P2 project is discussed. In Section 3 the workflow is presented in more detail, explaining individual simulation steps needed to achieve the desired output of the use case.

In Sections 4 and 5 the progress and next steps are presented. At the beginning, the achievements up to M12 are summarized. Then the progress since M12 is presented with focus on the development of two large-scale cases and optimisation of the codes used in the workflow. The Next Steps section contains the work layout for the future.

Table of Contents

Table of Figures

Table of Tables

1 Use Case Introduction

Fusion energy, as stated by F4E, European Union organisation managing Europe's contribution to ITER [1], *"offers the promise for abundant, safe and sustainable energy for the future"*. To contribute to the fulfilment of this promise, further ground-breaking developments with respect to reactor design but also with respect to reactor operation are necessary. To this end, UL is expected to conduct the setup of a digital twin of the first wall of a tokamak fusion reactor. This use case will not only contribute to the design and optimisation of this crucial part of a tokamak type fusion reactor by better explanation of the physical processes around the inner wall during the fusion reactions but also pave the path towards real-time control of fusion reaction, which is needed for stable fusion.

In this use case, an attempt at the setup of a digital twin of the first wall of a tokamak fusion reactor will be made. During the fusion reaction in a tokamak, determining the real temperature at the surface of the first wall of the tokamak from infra-red (IR) cameras is a crucial task for appropriate engineering design of the first wall and for later monitoring, while the fusion reaction is running, to detect in real time overheating parts and therefore, react before these parts of the reactor are damaged. To this end, the performance of the engineering parts of the tokamak (dependency on geometry and temperatures in the system) are modelled first with field-line tracing for magnetically conducted particles which contribute most to the power deposition to the first wall and a thermal model with Finite Element Methods and with Finite Volume Methods, i.e., via OpenFOAM. The results are expected to be validated using experimental data available from ITER first plasma experiments (using a temporary limiter) and WEST [2] (CEA tokamak), along with synthetic diagnostics that combines IR and visible light camera images.

The optical performance of visible light and IR cameras is simulated, based on Monte Carlo methods using forward ray-tracing algorithms to predict the optical flow. Optical parameters such as surface reflectivity are modelled with Cook-Torrance models, which are assessed with ray-tracing codes (Raysect [3]). An example of predicted camera output is shown below:

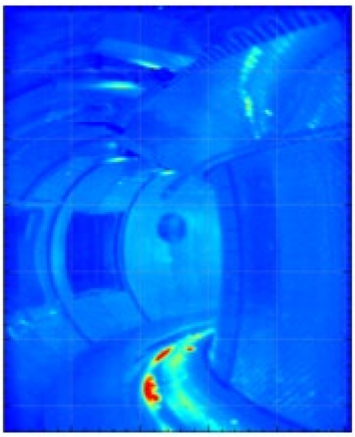

Figure 1: Synthetic camera image of WEST tokamak during operation.

2 Objectives of the Use Case

The goal of the use case is to accurately predict stray light, hot spots and uniformity to ensure performance and evaluate illuminance and luminous intensity in the visible and IR light range. The coupled thermal-optics simulations under high reflectance are used to correctly describe the visible light in cameras that see not only surface temperature but also reflected light from other surfaces. When reflections are subtracted, correct surface temperatures are determined. Therefore, only complete simulations (digital twins) can give the correct results, comparable to experimental IR camera measurements. The ray-tracing and thermal models of cooled surfaces are exascale relevant simulations with good scaling prediction. The inverse problem, when having a real camera image from which we would like to determine surface temperatures, knowing that the surfaces are reflective, can be only solved by having previously conducted forward simulations and taking some AI correlation algorithms to determine the correct heating scenario. The latter case is actually a requirement for real-time control of the engineering system. For this problem FPGA and accelerators is a perfect technology for real use cases.

It is the ambition of UL as the owner of the further application use case to advance beyond the state of the art with the setup of a digital twin and consequently the engineering design of the first wall of a tokamak type fusion reactor. This will be achieved by moving the coupled application of the community code OpenFOAM and Raysect towards more detailed simulation setups and more efficient workflow execution to acquire simulation results that will better explain physical processes around the inner wall during the fusion reactions.

UL prepared a small-scale use case which was simulated on the Slovenian peta-scale system VEGA and is now moving to large scale simulations based on the presented codes. To this end, UL, who was not part of the consortium during EXCELLERAT P1, but was informed about the work done via its participation in the interest groups, joined the consortium via the EXCELLERAT on-boarding, use case development and use case monitoring processes. These processes ensure proper integration of UL or any other new consortium member into the established EXCELLERAT P2 consortium and include assessment of the use case requirements, use case development in the respective tasks of the technical WPs as well as knowledge and competence exchange and progress monitoring.

3 Workflow Description

The accurate assessment of synthetic images requires three principal numerical simulations whose execution needs to be performed in sequence. The field-line tracing solver's output is an input to the thermal model and the thermal model's output is an input to the optical simulation which in the end returns results in the form of synthetic measurements, i.e., images. This simple scheme is sketched in Fig. 2.

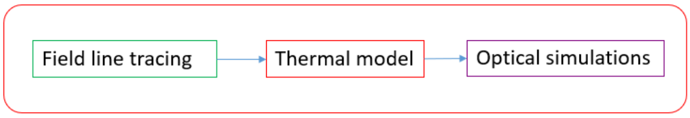

Figure 2: Sequential execution of codes for digital twin.

For field-line tracing and thermal modelling, the geometry components are independent of each other and they are easily parallelizable. For simple definitions of first wall geometries (components with trivial shaping with no need for much detail, components which are not actively cooled, …) the assessment of heat fluxes and temperatures is expected to be delivered faster than more complex shapes such as actively cooled components with complex shapes such as different castellations etc. However, for an optical simulation a full temperature distribution is needed in order to give accurate results. Along with large input and output data, there is a significant challenge for an appropriate coordination of the computational resources (different hardware and queue system).

For simulations and post-processing, it is planned to first test the VEGA system through development access mode. As mentioned above, the described modelling work has been partially done at the University of Ljubljana even though the executed simulations were limited and the produced results had lab type character. Therefore, UL will follow the classical task path:

- getting access to a peta-scale system (VEGA),
- deploying code and data to the system,
- preparing and running the simulations by porting the workflow and moving it to larger scales,
- evaluating and validating the results.

After that UL will introduce significant workflow improvements to reduce time to solution and work towards the solution of the real time problem.

The workflow is depicted in Fig. 3:

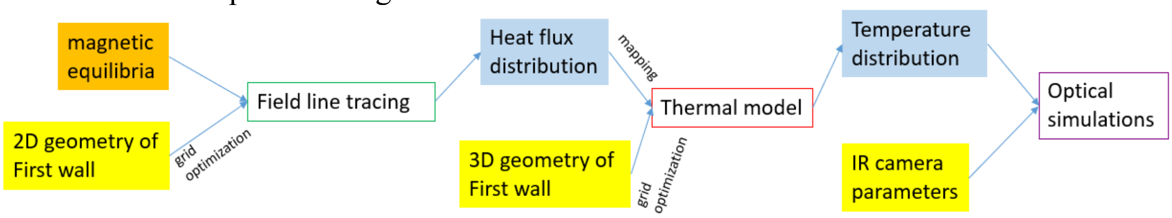

Figure 3: Workflow components for the simulation of a digital twin that outputs IR camera images.

For the field-line tracing part, the magnetic equilibria inputs (information about magnetic field, magnetic flux, plasma power etc.) will be supplied to UL from partners at ITER and CEA. UL has a collaboration agreement with both parties for the length of the EXCELLERAT P2 project and has access to the databases containing these inputs. For the optical simulation part, the current available camera design will be supplied by CEA which is responsible for the design of camera in ITER as well. The camera parameters will include camera position and geometry (with focus on CCD sensor and aperture), including corresponding field of view, and spectrum range. Additional parameters will be reflectivity coefficients to properly simulate reflections. To optimise the workflow the inputs and output data between different simulation steps will be stored in appropriate data format (HDF5, netCFD, …).

4 Progress achieved since M12

The three simulation steps are assessed with the following codes:

- L2G (field-line tracing)
- OpenFOAM (thermal modelling)
- Raysect (optical simulations)

In milestone M12 report, a small-scale case was presented by FA-1, focusing on a block of a temporary limiter inside the ITER reactor. With this small-scale simulation, we demonstrated the execution of the full simulation workflow of field line tracing – thermal model – optical simulation. The case itself simulates individual graphite block which was at the time meant to be installed for ITER first plasma testing. The magnetic equilibrium consists of 48 time steps with size of 0.4s, defined on structured R-Z grid of size 65x129 nodes, assuming axisymmetry in Φ direction. The approximate size of graphite block was 1m x 0.m x 0.3m. The size of front plasma-facing surface used in field-line tracing simulation was ~32k triangles. Thermal model simulated with OpenFOAM consisted of ~300k tetrahedrons. Shadow geometry to assess which field-lines have been blocked and do not connect from plasma to the target geometry, consisted of ~500k triangles. At that time, the L2G (field-line tracing) and Raysect (optical simulations) codes were parallelised only within a single node, providing an initial validation of the computational approach.
Since M12, progress has been made both in terms of expanding the physical models and improving computational efficiency. Two large-scale simulation cases have been prepared. One case targets the WEST reactor at IRFM, CEA Cadarache, offering a more complex and realistic experimental environment, that can be compared to experimental results (Fig. 4 and Ref. [4]). The second case is focused on modelling the actively cooled first wall panels that are supposed to be installed in ITER.

L2G code solves the standard field-line tracing equation:

$$\frac{dx}{dt} = B(t)$$

The parameter t can be understood here as a pseudo-time measured along the field-line and identifies the size of field-line step. The algorithm calculates magnetic field B at each target triangle (target mesh in this context represents the component that we are analysing) and then moves in the direction of the magnetic field for the defined step. Intersection with triangles that define neighbouring geometry is calculated. Then the procedure is repeated, until the field-line reaches the outer midplane of the plasma (where the power originates from). If field-line is intersected before it reaches the midplane, target triangle is considered to be shadowed from the plasma by the neighbouring components and thus receives 0 heat flux. In case of no intersection, different decay profiles are used to assess energy decay along the field line base on plasma power, from which heat flux can be calculated.

OpenFOAM package is used for thermal modelling. Our customised solver is based on the laplacianFoam, and was modified so that spatial heat fluxes and temperature dependent material properties and heat transfer coefficients can be taken into account. Spatial discretisation is second-order accurate in space, and a Crank–Nicolson time-stepping scheme is used in time. The system of equations can be solved with different solvers (CG, BiCGStab, GAMG, …) and preconditioners (DIC, DILU, AMG) available within OpenFOAM. Parallelisation is achieved via domain decomposition with scotch and MPI communication.

Raysect uses a Monte Carlo forward ray-tracing algorithm. For each pixel a set of rays is launched into the scene, until they hit an emitting surface or some termination criterion is reached. The core ray-tracing routines are implemented in C and exposed via a Python interface.

WEST case was focused on lower divertor baffle and ICRH antenna bumper (see Fig. 5). 3D magnetic field, accounting for ripple effects and thus defined on R-Z-Φ grid with ~100k cells in total. Target geometry (bumpers + baffl) comprised of ~3million triangles. 3D mesh was defined with ~2m tetrahedrons. Both geometries are passively cooled components. Boundary condition is heat flux from plasma and zero heat flux elsewhere, except at the bottom where 110°C due to nearby cooling channels (which are not included in the simulation). The camera is defined with 500x500 pixels with 1000 rays per pixel and checked for intersection with both of the components studied in our case. For other components we assume low constant temperature similar to coolant to assume they don't radiate too much. This is true for some of the components in the reactor, in particular for the outer wall that is far away from the plasma (compared to bumpers and baffle). This is not the case, however, for upper divertor and some plates on the inner wall (see Fig. 5). In the remaining time of the project, we plan to expand the case and include these components as well.

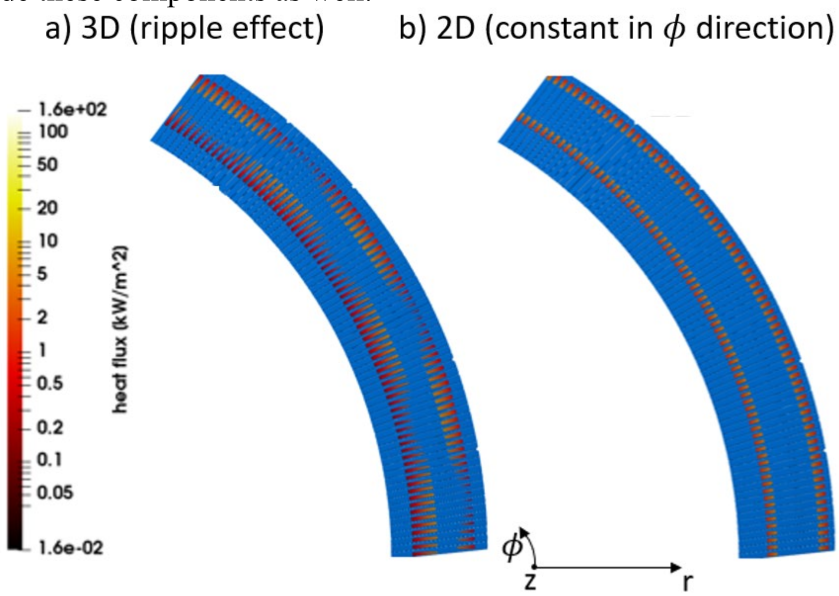

Figure 4: Effect of magnetic ripple effect on divertor (a), compared to magnetic field constant in ϕ direction (b). For location of divertor in WEST and its ripple pattern of heat flux, see Fig. 5(a).

In terms of physical phenomena, all three codes have been improved. For field-line tracing (L2G code), the model now simulates magnetic field disruptions in ϕ direction (see Fig. 1a). Although in theory, the magnetic field is constant in ϕ direction, a so-called magnetic ripple effect can appear due to different events, for instance misalignment of magnetic coils caused by their own weight, changes in electric current etc. These effects are now accounted for (see simulation result in Fig. 4a and experimental image in 5a).

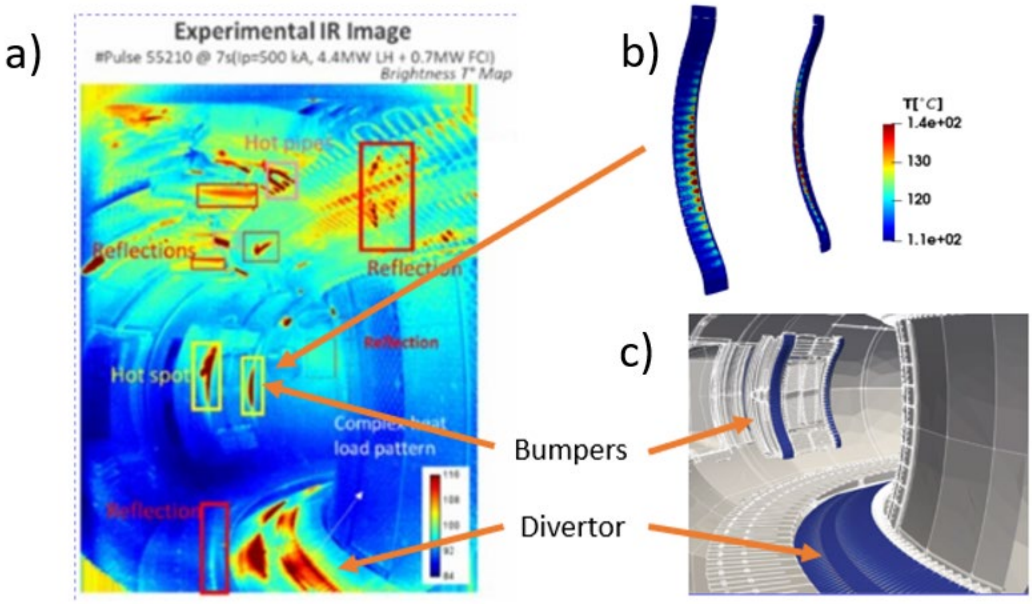

Figure 5: (a) Experimental measurement of IR camera in WEST reactor (figure courtesy [4]) (b) Temperature distribution on bumper of ICRH antenna heating unit (c) Location of bumper and divertor in WEST reactor

ITER panels are defined with so-called castellation – W or Be cubes, attached to subcomponents with coolant sink (see Fig. 6c). For panel 4, which is expected to be one of the most heavily loaded components, there are 6300 of such cubes. For thermal modelling, the 3D model has been extended to take into account multiple material properties. For example, a panel in ITER is composed of different materials – W, CuCrZr, and stainless steel, see Fig. 6c. This gives us the possibility to define properties of coolant and model actively cooled components in more detail.

In ITER case, one poloidal loop was studied (shown in Fig. 6a – panels that define a loop in R-Z plane from 1 to 18 and are constant in Φ direction). This poloidal loop was defined with ~600k triangles (without taking into account all the cubes, but rather approximate analytical surface spanning across the cubes). In total there are 18 such loops around the panel (one panel occupies ~20°), so shadowing geometry was defined with $18 \times 600k \sim 10$ million triangles. Magnetic equilibrium was defined on structured R-Z grid with 257 x 513 nodes and assumes diverted plasma, approaching to the inner wall towards panels 3,4 and 5. Front surface, exposed to plasma, is subjugated to heat fluxes, assessed with the 1st step of the workflow (field-line tracing simulation). The boundary condition on the front surface of the 3D model is thus spatial and time dependent heat flux. Other outer surfaces are set to adiabatic boundary condition and the surfaces of the cooling channel are defined with $T_{coolant} = 110$°C and temperature dependent heat transfer. 3D model consisted of 9 million triangles. All materials, comprising the 3D model, are temperature dependent. For optical simulations, radiation from surfaces has been modelled with the Stefan-Boltzmann law, taking into account the full reactor with the same size as shadowing geometry (10 million triangles) The camera is assumed to have 100x100 pixels. From each pixel 100 rays are spawned into computational domain and checked for intersection with the reactor's surface. Then the power arriving at the pixels is assessed through non-time-consuming calculation based on surface temperature.

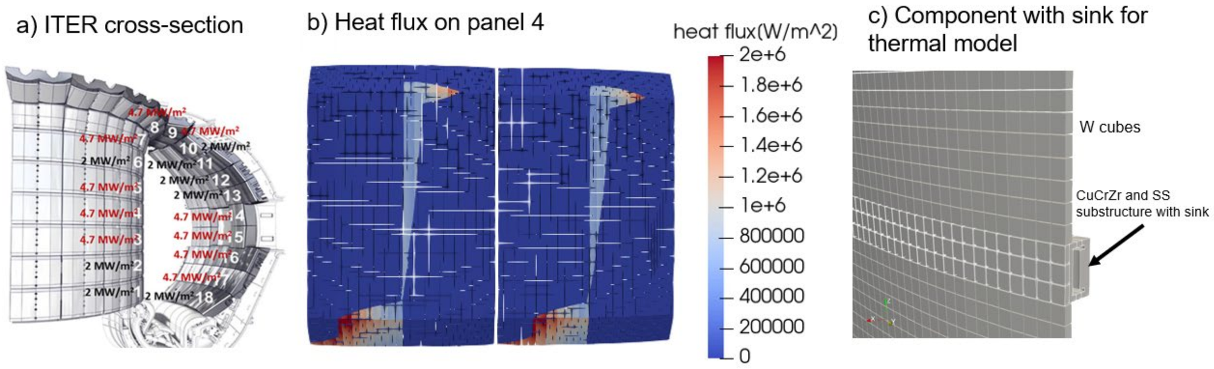

Figure 6:(a) Cross-section of ITER in R-Z plane (b) Heat flux on castellated panel 4, modelled with L2G (c) Substructure of panel 4, used for thermal modelling of active cooling in OpenFOAM.

Effort has also been invested to optimise the workflow. Field-line code L2G and optical simulation code Raysect have been extended to distributed memory architectures with the OpenMPI library. An initial performance study of L2G on the Vega supercomputer revealed encouraging scalability results. The time required for serial execution was approximately 16 minutes, while distributed parallel execution using 5,000 cores reduced the simulation time to just 24 seconds. OpenFOAM simulation of ITER panel 4 running with 1200 processes reduced computational time from ~58 minutes in serial to 16 seconds. Raysect required ~228 minutes in serial execution and was reduced down to ~22 minutes running on 1560 processes. These results are explained in more detail in D3.2. Although results already demonstrate a substantial speedup compared to shared memory architecture use only, further optimisation efforts are needed to enhance scalability, particularly as simulations move towards exascale computing environments.

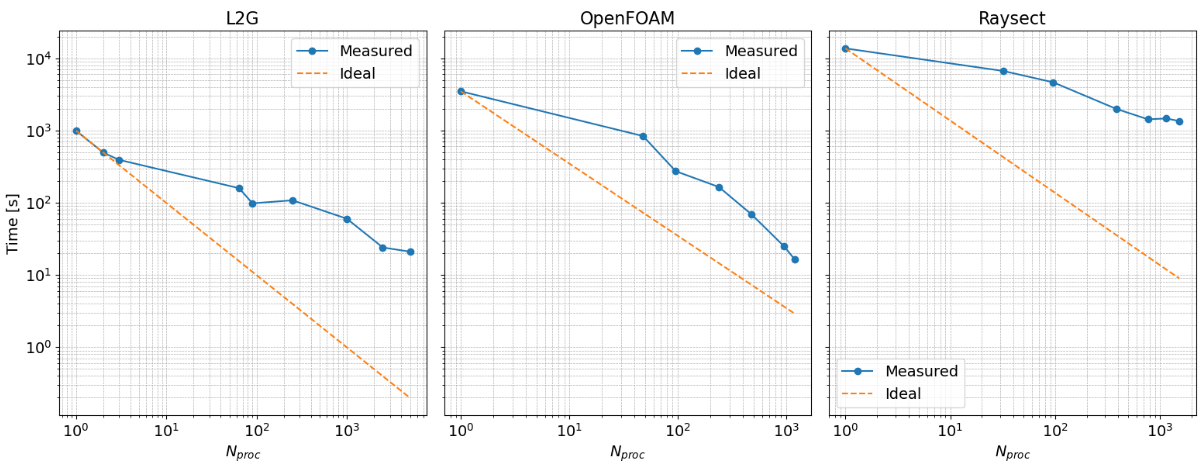

Figure 7: Strong scaling plots for all FA-1 codes.

The complexity of the FA-1 workflow is due to different formats of input and output files for the three codes used within FA-1. The UL team has been developing a simple Python library that enables users to easily setup their own cases without heavy interference with allocating jobs on a HPC system. Table 1 encompasses key aspects of all three simulations.

	Field line tracing (L2G)	**Thermal model (OpenFOAM)**	**Optical simulation/ray-tracing (Raysect)**
Pre-processing, Simulation runs Post-processing	Input **yaml** file, geometry modified in **SALOME platform**	L2G output processed with **Python** to create input files, geometry	OpenFOAM output processed with **Python** to prepare temperature for Raysect
Manual effort/automatic procedure	User modifies and executes **yaml** file, in which magnetic field (ASCII/binary format) and geometry (**MED** file format) is specified	User prepares CAD models and meshes which are called by **Python** to prepare the case and execute it.	The same meshes as in field line tracing, camera defined in **Python**, which then also generates batch script and executes it
Tools/libraries/codes/ numerical methods involved	Interface in **Python,** Kernel written in **C,** Numerical method is field-line tracing	Standard libraries that are part of OpenFOAM Numerical method is FVM	**Python** interface, kernel written in **C** Hybrid parallelisation (**OpenMPI** + **multiprocessing**), numerical method is ray-tracing

Table 1: Overview of three simulations used in FA-1 workflow.

5 Next Steps

UL will focus on two goals: improving scalability and completing both case studies to produce synthetic diagnostic outputs. For the WEST reactor, the goal is to expand beyond bumpers and divertor targets and include the full reactor. For the ITER scenario, the inclusion of actively cooled first wall panels will be finalised so that geometrical and material complexities are properly modelled. These completed simulations will then be used to generate synthetic camera signals with optical simulations, enabling the creation of virtual diagnostics that mimic the response of infrared (IR) imaging systems. This will support validation of the models and prepare the workflow for comparison with experimental data.

More effort will need to be invested across all three simulation components: field-line tracing, thermal modelling, and optical ray-tracing. Although current implementations already support distributed memory architectures and exhibit measurable speedups, further optimisation is necessary to fully exploit high-performance computing resources, particularly in anticipation of using exascale computing platforms. Efforts will target improved load balancing, memory efficiency and parallel input/output operations.

6 References

[1] "ITER - the way to new energy," ITER. Accessed: Oct. 13, 2022. [Online]. Available: http://www.iter.org

[2] IRFM CEA, *WEST tokamak*. Accessed: Jan. 06, 2023. [Online]. Available: http://irfm.cea.fr/en/west/

[3] Carr Matthew and Alex Meakins, *Raysect Python Ray-tracing package*. [Zenodo]. Available: https://doi.org/10.5281/zenodo.1205064

[4] Aumeunier M.-H. et al, Infrared thermography in metallic environments of WEST and ASDEX Upgrade, 2021 Nucl. Mater. Energy 26 100879