Code Integration, Data Verification and Models Validation using the ITER Integrated Modelling and Analysis System (IMAS) in EUROfusion

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Abstract

The ITER Integrated Modelling and Analysis System (IMAS) has been adopted by the EUROfusion consortium as a platform to facilitate the analysis and verification of data from multiple Tokamaks, for the integration of physics codes and the validation of physics models for fusion plasma simulations. Data mapping tools have been developed to translate the Tokamaks native data format into IMAS. The mapping required adoption of standard coordinates, conventions on direction of vectors, signs of fields and harmonization of physics units. The mapped data have been verified by running integrated simulations using Kepler workflows. Results of the test using IMAS data are reported here along with an assessment of the System for present and future fusion applications.

1. Introduction

EUROfusion is a consortium of institutes and laboratories coordinating the fusion programme on behalf of the European Commission with the aim of delivering the European Fusion Roadmap [1]. EUROfusion is currently utilising five different Tokamaks JET, TCV, AUG, MAST-U and WEST [2,3,4] to carry out its research plan in support of ITER and in preparation for DEMO. Work in EUROfusion is highly collaborative and analysis of the data from the above devices by internationally distributed scientists requires a high degree of standardization and the development of a common data platform. The EUROfusion project Code Development for Integrated Modelling (CD) [5] is in charge of delivering a unified data system and standards for code integration along with workflows for data analysis, code verification and validation. The activity of CD stems from the pioneering work done by the

European Task Force Integrated Tokamak Modelling (ITM) [6]. The choice of CD is to fully embrace the ITER Modelling and Analysis System (IMAS) based on the Interface Data Structure (IDS) [7] for EUROfusion Tokamak-data standardization and code integration. A new coordinated activity started in 2019 involving data experts of all the EUROfusion Tokamaks to develop tools for the mapping of experimental data in IMAS / IDS. A EUROfusion virtual laboratory is being built on the European Gateway cluster [8] to host the data in IMAS format (IMAS database) along with analysis and modelling tools all IMAS compatible. Three workflows are ready for the verification of the experimental data and models validation: the equilibrium reconstruction workflow (EQRECONSTRUCT) [9], the MHD stability workflow and the European Transport Simulator (ETS) [10]. The European Transport Solver (ETS) integrates several physics modules that span from advanced first principle transport models to heating and current drive models, pedestal models, atomic and nuclear cross sections, impurity transport models, SOL and divertor modules. All these modules have been integrated in ETS on a single platform using IMAS and therefore it offers a comprehensive overview of different aspects of code integration. A campaign for model validation using the CD workflows has been launched within the experimental programs of the various EUROfusion Tokamaks. In the next section we describe the ITER data structure and the mapping tools. In section 3 we describe the code integration and the IMAS workflows. In section 4 we present the results of the data verification and models validation.

2. Mapping of EUROfusion Tokamak data in IMAS / IDS

The backbone of the IMAS is the data model currently made of 55 datatypes defined by the IMAS Data Dictionary, a set of XSD specification files. Each datatype is a so-called Interface Data Structure (IDS) related to the description of a sub-system like a diagnostics or a

conceptual entity grouping a set of physical quantities. For example, we find the 'interferometer' IDS which is related to the interferometry diagnostics and the 'equilibrium' IDS which is a complex structure that contains all the data related to the calculation of the plasma equilibrium such as the pressure profile, the current profile, the safety factor profile, the two-dimensional map of the poloidal flux and more. In order to illustrate this concept an extract of the structure of the IDS 'equilibrium' is illustrated in Table 1.

Full path name of each node	Node description	Data type
time_slice(itime)/boundary/psi	Value of the poloidal flux at which the boundary is taken {dynamic} [Wb]	FLT_0D
time_slice(itime)/boundary/geometric_axis	RZ position of the geometric axis (defined as (Rmin+Rmax) / 2 and (Zmin+Zmax) / 2 of the boundary)	structure
time_slice(itime)/boundary/geometric_axis/r	Major radius {dynamic} [m]	FLT_0D
time_slice(itime)/boundary/geometric_axis/z	Height {dynamic} [m]	FLT_0D
time_slice(itime)/boundary/minor_radius	Minor radius of the plasma boundary (defined as (Rmax-Rmin) / 2 of the boundary) {dynamic} [m]	FLT_0D
time_slice(itime)/boundary/elongation	Elongation of the plasma boundary {dynamic} [-]	FLT_0D
time_slice(itime)/boundary/elongation_upper	Elongation (upper half w.r.t. geometric axis) of the plasma boundary {dynamic} [-]	FLT_0D
time_slice(itime)/boundary/elongation_lower	Elongation (lower half w.r.t. geometric axis) of the plasma boundary {dynamic} [-]	FLT_0D
time_slice(itime)/boundary/triangularity	Triangularity of the plasma boundary {dynamic} [-]	FLT_0D
time_slice(itime)/boundary/triangularity_upper	Upper triangularity of the plasma boundary {dynamic} [-]	FLT_0D
time_slice(itime)/boundary/triangularity_lower	Lower triangularity of the plasma boundary {dynamic} [-]	FLT_0D

Table 1. Extract from the list of nodes contained in the equilibrium IDS. FLT-0D indicates a floating point variable of dimension 0 (a real number). The data type 'structure' will have sub nodes as illustrated in the table. The keyword "dynamic" indicates that the value can change at different times (itime).

Together with the IDS 'equilibrium' the IDSs released by ITER so far cover most of the common Tokamak diagnostics and analysis / simulation data in use. The list of all the IDSs together with their documentation can be downloaded the ITER confluence site [11] by developers / users with an ITER account. A set of libraries and low-level routines (Universal Access Layer) for reading and writing IDSs and for the definition/allocation of IDS type variables in simulation codes is provided by ITER as part of the IMAS environment. The definition of the IDSs constitutes the ITER data format which provides a solution for the standardization of fusion data. It carries also a series of conventions on physics units, direction of arrays, definition of angles and signs of fields. The present version of IMAS adopts the COCOS=11 convention [12]. A novel tool has been developed for the mapping of EUROfusion data in IMAS, the Universal Data Access (UDA) component. This is a generic client/server solution which can be adapted to a machine by providing a specific plugin to the server. At the time of writing, the UDA project provides one plugin for each EUROfusion machine. Every time a UDA client requests a specific field contained in an IDS for a specific machine, the server forwards the request to the plugin associated to this machine. Running on the server, UDA plugins have generally access to raw data measured by diagnostics, machine description data, and also processed data produced by computation programs. These data are generally found in flat files or SQL databases, provided by current available technologies like for example MDS+ or HDF5 servers. The plugin retrieves the wanted data using the available information to map the request. Finally, IMAS users utilise UDA for sending bunches of

requests to build IDSs objects on the client machine. From the user point of view, IDSs objects obtained from UDA behave exactly the same as they were obtained from a local access.

At the time of writing, the EUROfusion-data mapped with UDA include the following IDSs: bt, magnetics, pfcoils, iron core, MSE, Thomson Scattering. More complex is the mapping of data into the core_profile IDS. The above IDS includes the electron and ion temperature and density profiles versus rho_thor (reference radial coordinate) mapped onto the plasma equilibrium. These data are not routinely available in Tokamak databases and require pre-processing of raw diagnostic data. The mapping of data in the core_profile IDS has been carried out with different technologies for different Tokamaks. For TCV a set of MATLAB routines has been provided while for AUG a tool used for setting up transport simulations (TRGUI) has been modified to write data in IMAS (TRVIEW). Finally, for JET and MAST a novel OMFIT [13] module has been developed, called IMASgo, which builds upon the OMFITprofile and KineticEFIT modules [14, 15]. IMASgo allows to read the intershot equilibrium as well as pressure constrained equilibrium and maps the Thomson Scattering or ECE data on the flux coordinate. Fitting procedures are available for the generation of the plasma profiles. A representation of the IMASgo workflow is shown in Figure 1 and the electron temperature profile obtained fitting the MAST Thomson Scattering data mapped on the equilibrium is shown in Figure 2.

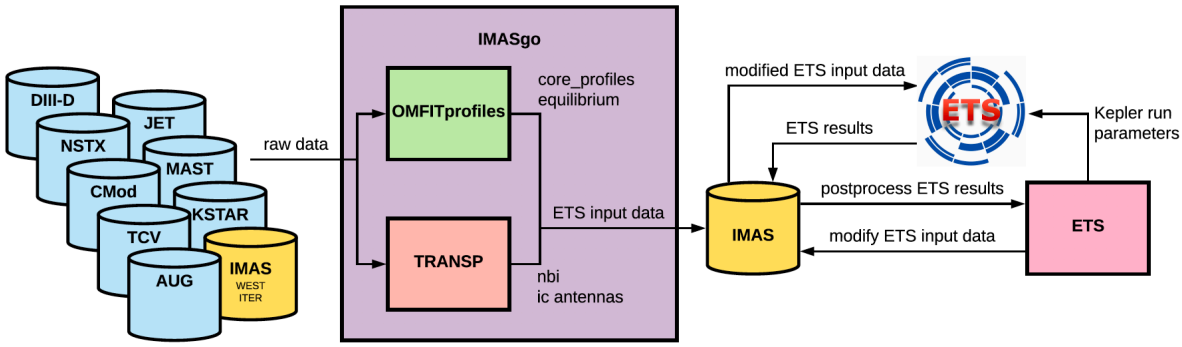


Figure 1. IMASgo allows to map data in IMAS that are not directly available in Tokamak databases such as the content of core_profile or the NBI / IC antenna IDSs

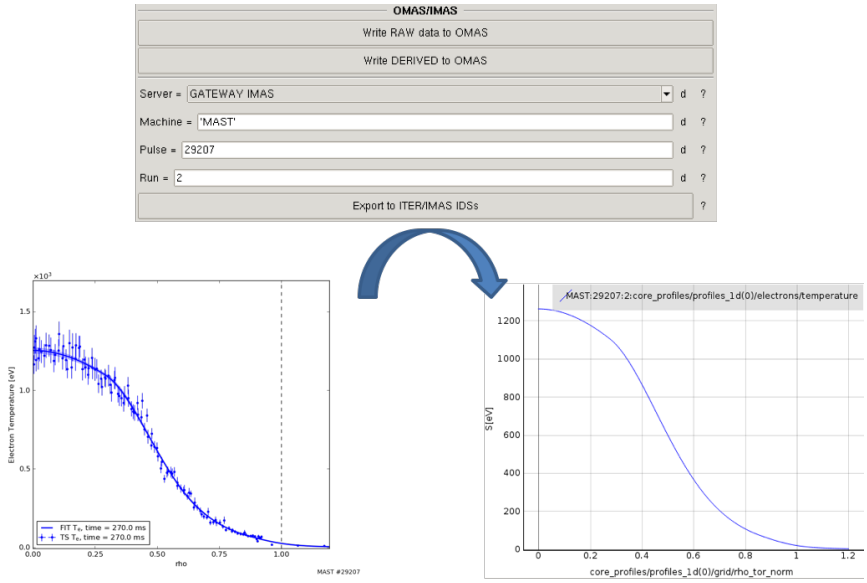
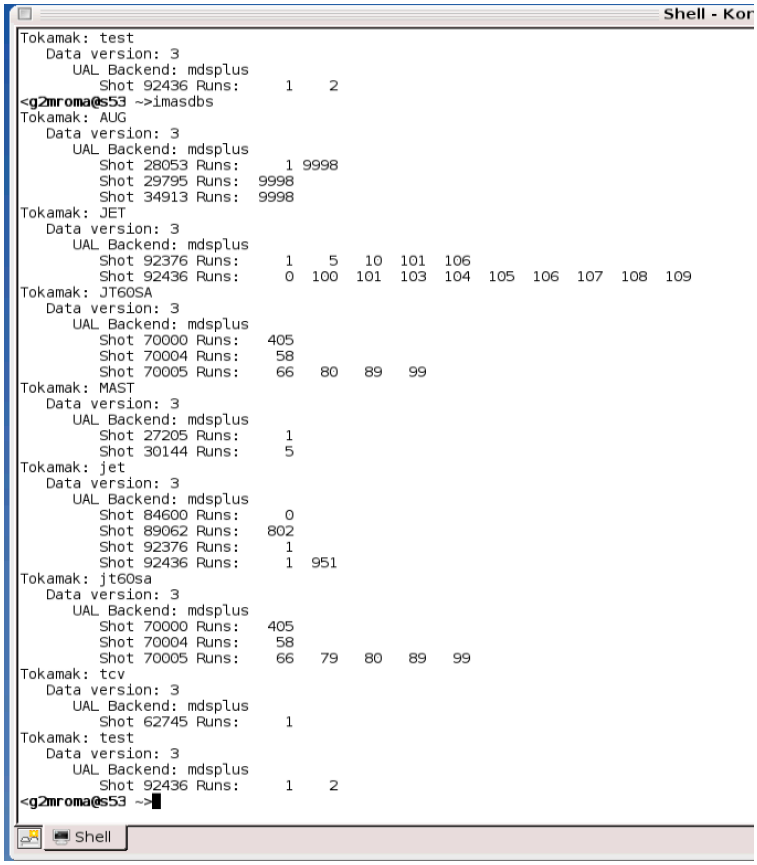


Figure 2. MAST Thomson Scattering data mapped on the equilibrium, fitted (left plot) and written into the core_profile IDS (right plot)

IMASgo utilises the information available in OMFIT for TRANSP to map the NBI and ICRH machine descriptions in IMAS. The mapping of data in IMAS goes through an intermediate step which utilises the OMFIT internal data structure (OMAS) [16]. The OMAS data structure is a one-to-one map of the ITER IDSs. The OMAS data are written into an IMAS

file on the Gateway. A snapshot of the IMAS database of one of the users of the Gateway is shown in Figure 3.



```
Tokamak: test
   Data version: 3
      UAL Backend: mdsplus
         Shot 92436 Runs:     1    2
<g2mroma@s53 ~>imasdbs
Tokamak: AUG
   Data version: 3
      UAL Backend: mdsplus
         Shot 28053 Runs:     1 9998
         Shot 29795 Runs:  9998
         Shot 34913 Runs:  9998
Tokamak: JET
   Data version: 3
      UAL Backend: mdsplus
         Shot 92376 Runs:     1    5   10  101  106
         Shot 92436 Runs:     0  100  101  103  104  105  106  107  108  109
Tokamak: JT60SA
   Data version: 3
      UAL Backend: mdsplus
         Shot 70000 Runs:   405
         Shot 70004 Runs:    58
         Shot 70005 Runs:    66   80   89   99
Tokamak: MAST
   Data version: 3
      UAL Backend: mdsplus
         Shot 27205 Runs:     1
         Shot 30144 Runs:     5
Tokamak: jet
   Data version: 3
      UAL Backend: mdsplus
         Shot 84600 Runs:     0
         Shot 89062 Runs:   802
         Shot 92376 Runs:     1
         Shot 92436 Runs:     1  951
Tokamak: jt60sa
   Data version: 3
      UAL Backend: mdsplus
         Shot 70000 Runs:   405
         Shot 70004 Runs:    58
         Shot 70005 Runs:    66   79   80   89   99
Tokamak: tcv
   Data version: 3
      UAL Backend: mdsplus
         Shot 62745 Runs:     1
Tokamak: test
   Data version: 3
      UAL Backend: mdsplus
         Shot 92436 Runs:     1    2
<g2mroma@s53 ~>
```

Figure 3. Snapshot of the IMAS database of a Gateway user accessed via the command imasdbs

Integrated Modelling Workflows

The adoption of standardized physical objects as input / output variables of physics codes allows for the interchangeability of codes inside complex simulation workflows. Three workflows have been developed by CD using the Kepler [17] integration framework. The first workflows developed using the above technology have been the equilibrium

reconstruction (EQRECONSTRUCT) which couples magnetic fitting equilibrium codes to fixed boundary, high-resolution codes and the MHD stability (EQSTABIL) which couples linear MHD stability codes to the high resolution equilibrium. Along with the EQRECONSTRUCT and EQSTABIL workflows, the European Transport Simulator [18,19] is the most complex of all the workflows and encompasses several physics modules spanning from heating and current drive modules, first principle transport models, pedestal models, edge transport modules etc. Figure 4.

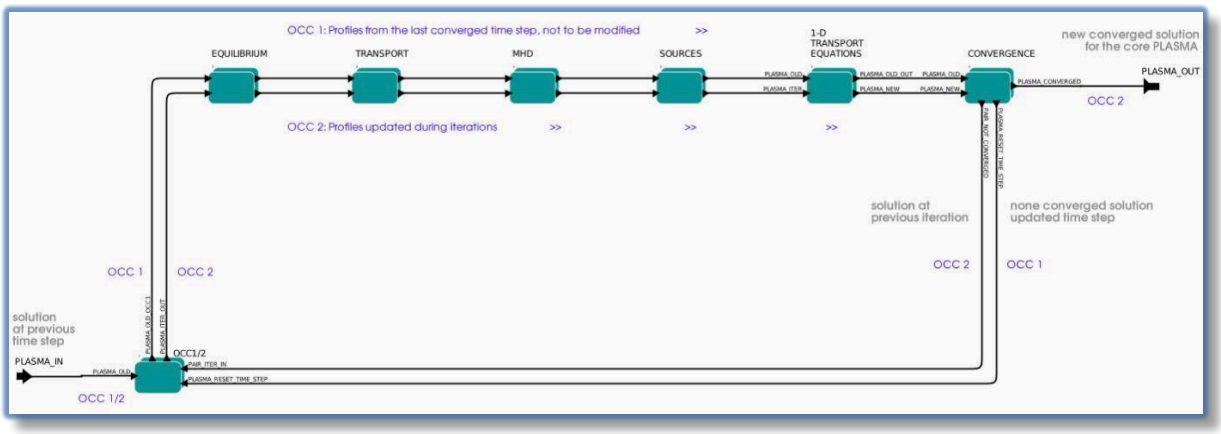


Figure 4. The ETS Kepler workflow integrating more than 50 physics modules including heating and current drive modules and first principle transport models.

The core of ETS is a 1.5-d transport solver designed and implemented within the integrated modelling framework. It can be run in interpretative as well as predictive mode and selectively evolve poloidal flux, ion densities (it can also be limited to an electron density solver), electron and ion temperatures as well as toroidal velocity restricted only by limitations in calculating corresponding transport coefficients and source terms. Impurities are solved for within a separate transport solver that is directly linked into the convergence loop. The solvers have been benchmarked and verified against other transport codes [19, 20]. ETS integrates more than 50 physics codes and modules (Kepler actors). Each of the physics

codes have been adapted to use consistent physical objects as input / output variables. ETS includes several equilibrium codes, the most advanced transport models and a state-of-the-art heating and current drive workflow.

Verification and validation of the IMAS data with EQRECONSTRUCT and ETS

Data mapped in IMAS can be visualised with IMASviz [21], a generic visualization tool for IDS-data made available by ITER. IMASviz allows to plot both profiles and time dependent data.

Magnetic data mapped in IDSs have been verified by running the EQRECONSTRUCT workflow. This allowed to identify and resolve issues with units and signs which were causing either the workflow to crash or to converge to a wrong solution.

By running EQRECONSTRUCT it was possible to verify the mapping of the magnetic data of all the EUROfusion tokamaks resulting in the workflow to be able to reconstruct correctly the equilibrium of all the Tokamaks after machine specific settings of the equilibrium reconstruction codes were identified. As an example, Figure 5(a), 5(b) show the equilibrium reconstruction from the magnetics IDS carried out for a TCV and JET plasma. This example consisted in running the equilibrium reconstruction with input only the data from the UDA mapping. During the process of verification, the equilibrium reconstruction workflow failed in several occasions due to: key data missing (not mapped by the responsible), incorrect units, incorrect signs, incorrect direction etc. The final result shown in Figure 5 is the converged equilibrium for TCV and JET which successfully verifies the data mapping.

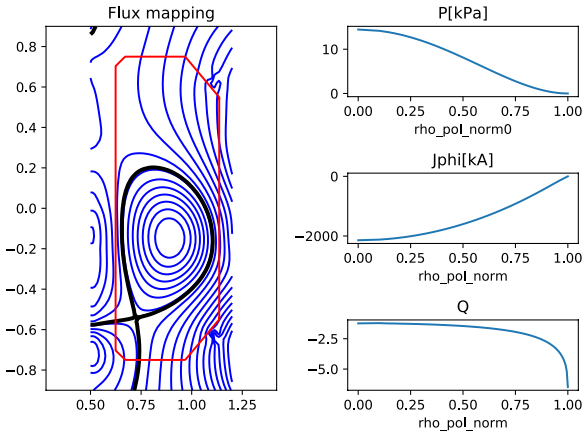


Figure 5 (a) TCV: R,Z [m] map of EQUAL equilibrium reconstruction at t=0.75s from UDA mapping for discharge #51262.

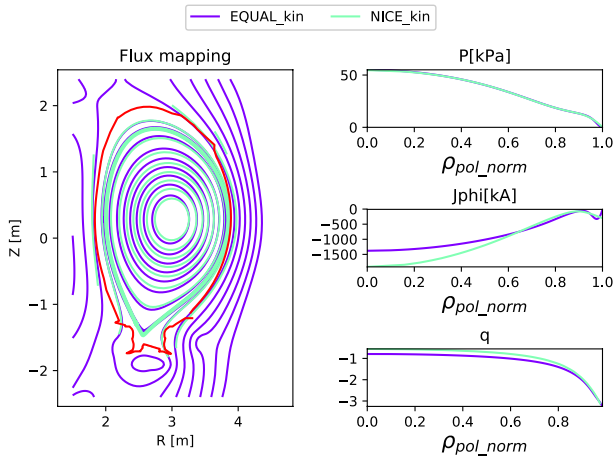


Figure 5 (b) JET: EQUAL and NICE reconstruction at t=51s from UDA mapping with pressure constraint for discharge #84600.

Data mapped in the IDSs containing the machine description of the NBI, ICRH, ECRH systems have been verified by running ETS and in particular the heating and current drive workflow. Visualization tools have been developed to verify the correctness of the heating systems configuration. Figure 6 and 7 show plots of the NBI IDS and the EC_antenna IDS for an AUG plasma (36757).

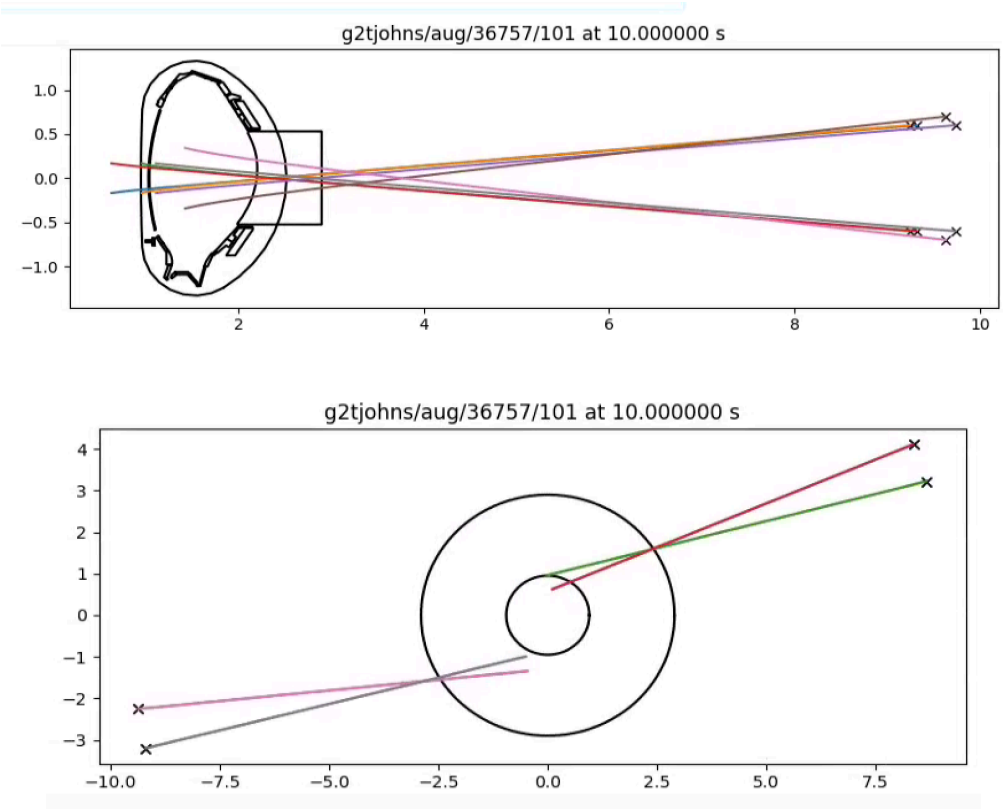


Figure 6: Plots of the WALL and NBI IDS of AUG for pulse 36757. Top chart: poloidal view (R,Z [m]); bottom chart: toroidal view (R,Y [m]). This visualization tool allows to verify the correctness of the data mapping in the NBI IDS.

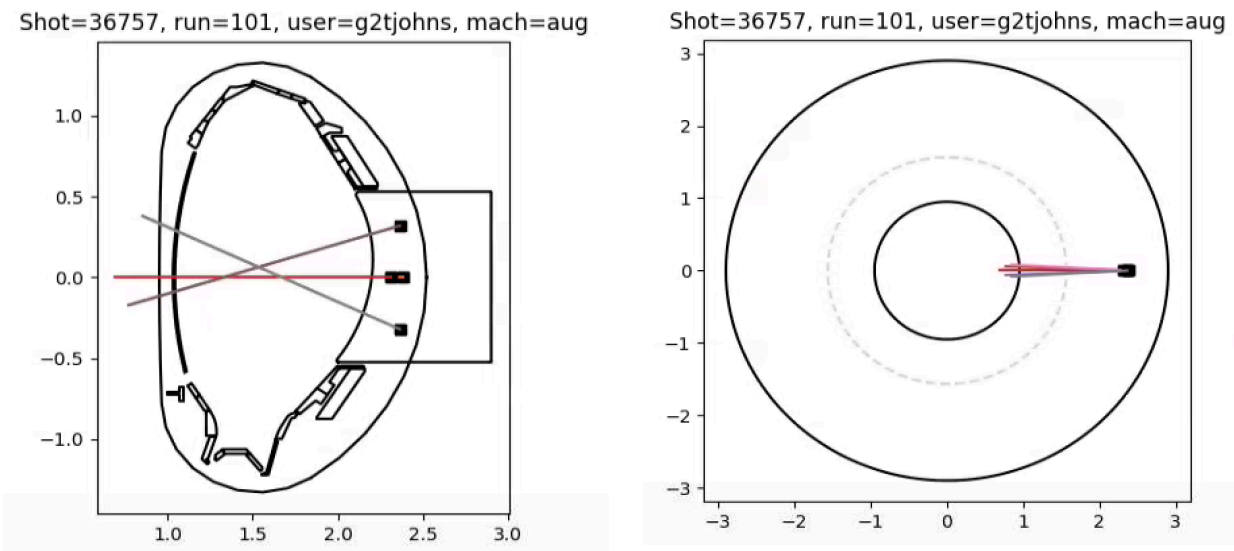


Figure 7: Plot of the WALL and EC_launcher IDSs for AUG 36757. Left chart: poloidal view (R,Z [m]) ; right chart: toroidal view (R,Y [m]). This visualization tool allows to verify the correctness of the data mapping in the EC_launcher IDS.

The content of the core_profile IDSs was verified by calculating the neutron rate with ETS and comparing it with the experimentally measured neutron rate from the neutron cameras. Figure 8 shows an example of such a verification for a JET plasma. The fast-fast and thermal-fast contributions have been calculated running the BBNBI / ASCOT codes with settings from the NBI IDS. The total neutron rate calculated is found to be within 10% of the measurement, within the error bar of the neutron cameras providing the validation for the neutral beam deposition module and the fusion cross sections.

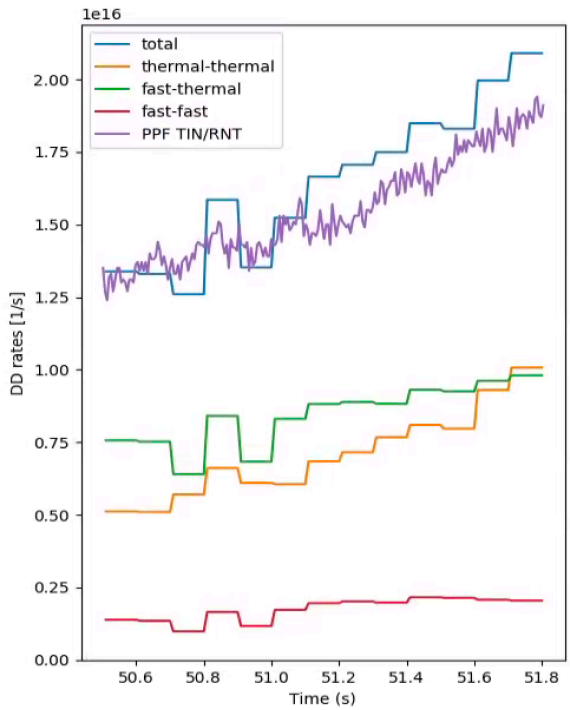


Figure 8: Comparison of the total neutron rate (blue) calculated with ETS from the input core_profile IDS of JET shot 94442 vs the experimental rate (purple). The fast-fast and thermal-fast contributions have been calculated running the BBNBI / ASCOT codes with settings from the NBI IDS

Conclusion

The need for analysing data from multiple EUROfusion Tokamaks and for applying the same set of analysis and modelling tools across the datasets required the definition of a standard for the data structure and code integration. Previous multi-Tokamak analysis have been made by exchanging ASCII and documentation files between users and lengthy and cumbersome porting of codes from one platform to another. Some codes were so rooted within a specific Tokamak environment that the porting would require rewriting substantial parts of the code. The ITER Integrated Modelling and Analysis System offers a platform for multi-Tokamak data-analysis verification and validation and for multi-code integration. IMAS has been adopted by EUROfusion for the analysis and modelling of data from its Tokamaks portfolio. Mapping tools have been developed for the conversion in IDSs of experimental data from their native format and integrated modelling workflows have been used for data verification and model validation. The routine use of the IMAS workflows across EUROfusion will provide continues model validation and code verification for the eventual exploitation at ITER. Overall IMAS has proven to be an effective tool and EUROfusion plans to continue extending its IMAS databases and set of IMAS workflows and analysis tools with the view of deploying it for ITER analysis. Standardised data will also be essential for future applications such as machine learning and artificial intelligence and IMAS is set to provide a powerful tool for model development / validation in view of ITER exploitation and for DEMO design.

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References

[1] A. J. Donné *et al* (2019), Roadmap Towards Fusion Electricity (Editorial). *J Fusion Energ* **38,** 503–505. https://doi.org/10.1007/s10894-019-00223-7

[2] E. Joffrin *et al* (2019) *Nucl. Fusion* **59** 112021

[3] H. Meyer *et al* (2017) *Nucl. Fusion* **57** 102014

[4] C. Bourdelle *et al* (2015) *Nucl. Fusion* **55** 063017

[5] M. Romanelli *et al* (2019) https://wpcd-workflows.github.io

[6] A. Becoulet *et al* (2007) Computer Physics Communications **177**(1-2):55 – 59.

[7] F. Imbeaux *et al* (2015) *Nucl. Fusion* **55** 123006

[8] B. Guillerminet et al (2010), Fusion Engineering and Design **85**, 410–41

[9] R. Coelho *et al* (2018), 27th IAEA FEC, TH/P5-27, IAEA CN-258.

[10] P. Strand *et al* (2018), 27th IAEA FEC, TH/P6-14, IAEA CN-258

[11] The IMAS Data Model, https://confluence.iter.org/display/IMP/Data+Model

[12] O.Sauter and S.Yu.Medvedev (2013) **Computer Physics Communications**, 184 (2) 293-302

[13] O. Meneghini *et al* (2015), Nuclear Fusion, Volume 55, Number 8

[14] N.C. Logan et al (2018), Fusion Science and Technology **74** (1-2), 125-134

[15] B.A. Grierson et al (2018), Fusion Science and Technology **74** (1-2), 101-115

[16] O. Meneghini, The OMAS datastructure, https://gafusion.github.io/omas/

[17] The Kepler project, https://kepler-project.org

[18] D. Coster *et al*, IEEE Trans. Plasma Sci. 38 (2010) 2085

[19] D. Kalupin *et al*, Nucl. Fusion 53, (2013) 123007

[20] Y-S Na, et al., (2016), 26th IAEA FEC, TH/P2-24, IAEA CN-234

[21] The IMASviz project, https://wpcd-workflows.github.io/IMASviz/index.html