INTEGRATED MODELLING & ANALYSIS SUITE: DEVELOPMENTS TO ADDRESS ITER NEEDS


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Abstract

The Integrated Modelling & Analysis Suite is the software infrastructure that is being developed to support the execution of the ITER Research Plan [1]. It builds upon expertise from across the research facilities within the ITER Members to create software that can be validated and applied to existing machines. The current focus is on developing predictive modelling capabilities to describe ITER plasma scenarios including all relevant physics processes and on preparing for experimental data processing and analysis. The paper describes recent developments in the underlying software infrastructure, physics model developments and applications.

1. INTRODUCTION

The Integrated Modelling & Analysis Suite (IMAS) is built around a standardised representation of data described by a Data Dictionary (DD) that is both machine independent and extensible. Machine independence is an important aspect since it allows tools and workflows developed in IMAS for ITER to be tested and refined on existing devices, whilst extensibility allows the DD to grow and evolve over time as more Use Cases are addressed. The use of standardised Interface Data Structures (IDSs) fosters the creation of modular physics components and (sub-)workflows that can be flexibly re-used to address different needs. Current development effort focuses on developing capabilities to make high physics fidelity predictive simulations of the plasma scenarios described in the ITER Research Plan and preparing for experimental data interpretation and analysis in advance of First Plasma.

2. IMAS INFRASTRUCTURE

The IMAS infrastructure is composed of various software elements that aim at simplifying the interactions between applications and the DD. Dedicated software covers IDS data access, generalized grids manipulation, data exploration and visualization, and generation of standardized components to be re-used in different applications or workflows. The most fundamental of these is the Access Layer (AL) which provides several ways to store and retrieve IDS data for a particular release of the DD, with interfaces in Fortran, C++, Matlab, Java and Python. Recent improvements to these AL interfaces include a new MEX-based Matlab interface offering improved performance compared with the previous implementation and a new Python AL interface which dynamically interprets the DD at runtime. This latter development has led to a much increased flexibility with regard to working with data represented according to different versions of the DD. It uses just-in-time reading of the DD definitions at runtime and allows datasets represented according to different DD versions to be imported at the same time. The new interface has been extensively tested against the current storage backends and performance optimized by reducing unnecessary allocations, smart memory usage and caching, and through manual optimizations of hot code paths.

The DD itself has evolved through a strict release cycle to now contain 68 distinct IDSs, mainly through an increased ability to describe additional diagnostic systems. Additional metadata within the DD schema also enables transparent data-conversion between different DD versions, avoiding extra copies in memory. The latest release is 3.32.0. In terms of data storage, a new HDF5 backend has been developed that allows IMAS datasets to be efficiently stored in a self-describing portable binary format. The backend has a much improved memory footprint and also includes compression capabilities to further reduce the required storage.

3. HIGH FIDELITY PLASMA SIMULATOR

One of the focal points driving development within IMAS is the creation of a High-Fidelity Plasma Simulator (HFPS) that can be used to predict ITER plasma performance as well as to develop detailed plasma operation scenarios fulfilling various requirements and constraints. The DINA code [2,3] has been extensively used to validate the capability of the ITER poloidal field system to support the plasma scenarios foreseen in the ITER Research Plan. It includes a free-boundary equilibrium evolution solver implementing feedback control of the plasma current, position and shape, taking into account eddy currents in the vacuum vessel, as well as numerous engineering limits imposed on the coils, their power supplies, and plasma-wall gaps. The JINTRAC code [4] refines the physics description in the plasma core and also couples its behaviour with that in the plasma edge and scrape-off-layer (SOL). It can describe time-dependent plasma transport, heating, fuelling, and transient behaviour and divertor power loads.

Both the DINA and JINTRAC codes have been adapted to use the IMAS DD [5], and have been further modularised to allow exchanging IDSs with additional external physics modules to enable the incorporation of other higher-fidelity physics models. The first demonstrations of weakly coupled DINA and JINTRAC
simulations [6] were successfully performed for optimizing the ITER 15MA DT baseline scenario. These have initiated an activity to implement a more tightly coupled model, suitable for studying the nonlinear physics occurring during the evolution of free-boundary equilibrium, time-dependent plasma transport and various sources including heating and current drive. The foreseen outcomes of this development activity are an improved understanding of the interplay of physics mechanisms at various levels of complexity and co-simulation capabilities with the ITER Plasma Control System Simulation Platform (PCSSP) [7] allowing the application of integrated control to scenarios and contributions to the verification of the ITER Plasma Control System (PCS).

4. HEATING & CURRENT DRIVE

One such high-fidelity physics workflow [8] that has been developed over the last year by a combination of ITER Staff, ITER internships, ITER Scientist Fellows and voluntary contributions, is a comprehensive heating and current drive (H&CD) workflow that is capable of describing all of the ITER heating systems as well as synergistic effects between them [8]. This workflow exemplifies the IMAS integrated modelling paradigm and has driven further refinements in the IMAS infrastructure. The workflow builds upon the extensive earlier work carried out within the EUROfusion Work Package for Code Development and has been implemented in Python.

The internal structure of the H&CD workflow has been generalised to enable any kind of algorithm to be easily implemented allowing flexible modelling of H&CD processes as part of specific physics studies. One recent example is the study of the synergistic effect between NBI ions, fusion-born alpha particles and IC waves in ITER DT scenarios. It has been shown that for a 15MA/5.3T baseline DT scenario, applying 33 MW NBI D beams and 10 MW of ICRH tuned at 40 MHz for a central fundamental D heating, synergetic effects are present but modest (below 5%), while the RF-NBI synergy is more significant in helium plasmas of the ITER second Pre-Fusion Power Operation (PFPO-2) phase with hydrogen beams combined with fundamental hydrogen heating. This example shows the capabilities and strengths of the H&CD workflow and its components to simulate combined effects of NBI, fusion-born alpha particles, and ICRH, essential to accurately predict the performances of ITER plasmas for the various scenarios of the ITER Research Plan.

5. SCENARIO DATABASE

The IDS-based database of ITER scenario simulations is continuously expanding (there are currently 539 active datasets out of a total of 1226) and is used to support ITER design activities including assessments of the ITER heating systems and diagnostics. Recent additions include the set of SOLPS4.3 simulations of ITER edge conditions (> 200 cases) and JINTRAC simulations of ITER L [9] and H-mode [10] conditions, both of which rely on the Generalized Grid Description (GGD) to store complex geometry data. Moreover, the SOLPS-ITER code suite can output the solution state as a set of IDS either as a snapshot at the end of the run or at regular intervals throughout a run. The description of a SOLPS edge plasma solution includes the edge_profiles, edge_transport, edge_sources, radiation, and divertors IDSs, plus the underlying equilibrium and wall IDS data. All cases also include two metadata IDSs, dataset_description and summary which are used by database tools to quickly identify simulations of interest for researchers. A ParaView-based SOLPS-GUI tool allows for visualization of the complex 2-D data directly from the IMAS database.

6. ENERGETIC PARTICLE STABILITY

As the first fusion device to confine a plasma which is dominantly heated by fusion-produced alpha-particles, it is important to be able to model energetic particle stability in ITER. A workflow to assess the energetic particle (EP) stability of plasma scenarios on computational timescales that enable relatively extensive studies to be performed has been developed. The workflow is based upon the LIGKA [11] and HAGIS [12] physics codes and has initially been used to investigate the stability of ITER PFPO-2 hydrogen plasmas for various orientations of the heating neutral beams (HNBs) [13].
FIG. 1. Energetic particle beta profiles for three combinations of the ITER heating neutral beams: on/on, off-on and off-off axis. For comparison, the profiles for the ASDEXUpgrade off-off axis beam combination and JT-60SA are also shown.

The normalised pressure profiles for the three configurations of the beams considered (on/on, off/on, off/off-axis) are shown in Fig. 1. The particle-based EP distribution function is provided by the H&CD workflow described in Section 4 above (represented with a million markers) and is processed and projected into the LIGKA constants-of-motion space. The free-energy for driving instabilities comes from gradients in the phase space which can be observed in Fig. 1 to be both positive and negative. Changing the orientation of the HNBs from off-axis (black line) to on-axis (blue line) is seen to lead to a much steeper negative gradient in the core of the machine which can be expected to be destabilising.

The EP stability workflow is a time-dependent Python workflow that implements a hierarchy of physics models of varying degrees of physics fidelity and has corresponding run-times in the range of seconds to hours. The current implementation fully supports the determination of the stability of a wide range of Alfvén Eigenmodes (AE) including BAEs, RSAEs, TAEs and EAEs. Extensions to treat other types of perturbations are underway.

In Fig. 2 the results of a time-dependent run based on shot #100015, run 1 from the IMAS scenario database are shown. This is a 5 MA / 1.8 T hydrogen plasma in PFPO-2 simulated with the METIS code [14]. It has a density that is 90% of the Greenwald value, the energy of the beams are 745 keV (to avoid shine-through with H injection) and the total injected HNB power is 22.3 MW (in ITER, the beam power has to be reduced with its energy due to the beam perveance matching criteria). The frequency evolution of various AEs with toroidal mode numbers ~30 can be seen in the plot on the left-hand side during the plasma current ramp-up. On the right-hand side the radial location of the modes is shown indicating the role played by the flat q-profile region where q is just above unity and no AE are found with toroidal mode numbers below ~35.

FIG. 2. Left: Evolution of Alfvén eigenmode frequencies (stable and unstable) as a function of time during the ramp-up of a PFPO-2 H-plasma in ITER as calculated by the LIGKA/HAGIS workflow based on a predictive METIS [14] run (#100015,1; 5 MA/1.8T). All modes in the negative EP gradient region between 0.35 < rho_pol < 0.55 are shown. Right: The same dataset showing the evolution of the AE’s radial localisation with time. Regions of low AE density are related to regions of low magnetic shear close to q = 1.
7. DATA PROCESSING & ANALYSIS

In preparation for ITER operations, work has started on the development of experimental data processing and analysis pipelines. These are essential since in contrast to existing machines upon which they can be tested, on ITER they will form the only way to process raw experimental data for subsequent processing, analysis and interpretation. A key element of this activity to allow testing is dynamic access to existing experimental data in the form of IDSs. This has been enabled by the creation of local plug-ins that handle the reading and mapping of experimental data into IDSs such as have been created by EUROfusion for the EU MST1 and JET devices, and Korea for KSTAR. The (typically static) Machine Description metadata, which is also included in IDSs and enables the creation of device-generic workflows, must also be locally curated.

8. DIAGNOSTIC MODELS

Diagnostic models, often called synthetic diagnostics, that take given physics parameters, e.g. from previous scenario simulations, and use them to predict the signals that will be produced by a particular diagnostic have many uses. They can be used to make performance assessment of diagnostics during their design, test controllers by providing the necessary input signals as part of a co-simulation involving the High-Fidelity Plasma Simulator and the Plasma Control System Simulation Platform, or they can be used within analysis workflows to help determine the underlying plasma state that best explains the signals seen on multiple diagnostics.

There has been much progress in this area with strong interactions between ITPA groups, ITER interns, Monaco postdoctoral fellows, staff and collaborators. In particular there is now a growing set of synthetic diagnostics that fulfill the IMAS paradigm of using IDSs for their input/output that can be applied to various use cases. As an example, a new generic model has been developed for simulating the Toroidal Interfero-Polarimeter (TIP), Density Interfero-Polarimeter (DIP) and Poloidal Polarimeter (PoPola). The only difference between the models is the input geometry, read from various instances of the interferometer IDS stored in the Machine Description database, corresponding to the geometry of individual diagnostics. Fig. 3 shows an example of input kinetic profiles read from the IMAS scenario database and the TIP geometry read from the Machine Description database. Fig. 4 displays the resulting densities measured along each line-of-sight and the corresponding line-averaged density as measured by the TIP synthetic diagnostic. This model takes the equilibrium, core profiles and interferometer IDSs as input, and delivers the interferometer IDS as output. The code has been developed as part of an effort to evaluate the diagnostic coverage of L-H transition detection in the Pre-Fusion Power Operation phase.

![FIG. 3](image)

**FIG. 3.** Left figure: density profiles for various time slices taken from the IMAS scenario database for an ITER case at 5MA/1.8T simulated by the METIS transport solver. Right figure: Geometry of the TIP Lines of Sight taken from the ITER Machine Description database.
Another model recently developed describes the refractometry channel of the high-field-side reflectometer. The refractometer provides supplementary measurements of the line-averaged electron density. It takes the equilibrium, core_profiles and refractometer IDSs as input, and delivers the refractometer IDS extended by the simulated synthetic signal. It includes noise and latency estimates to facilitate testing the performance of the diagnostic together with the Plasma Control System. For this purpose, it has been integrated within the DINA-PCS workflow. Fig.5 shows the results of an analysis illustrating that the relative error on the measured electron density is lower when the signal from both the refractometer and the reflectometer are combined.

Models have also been developed for the Neutron Flux Monitor (NFM) and the Divertor Neutron Flux Monitor (DNFM). They take the equilibrium, distribution_sources and neutron_diagnostic IDSs as input, and deliver the neutron_diagnostic IDS as an output, including the simulated synthetic signal, namely the total neutron flux and fusion power. The DNFM and NFM diagnostics are respectively more sensitive to vertical and horizontal plasma shifts. An analysis has been carried out showing that combining the two delivers a measurement with less systematic error, as illustrated in Fig. 6.

**FIG. 5.** Relative error on the line-averaged electron density as evaluated by the refractometer only (left figure) and the combination between the refractometer and reflectometer (right figure).

**FIG. 6.** Comparison of uncertainty in total neutron flux and fusion power when the Divertor Neutron Flux Monitor diagnostic is used alone or combined with the Neutron Flux Monitor in equatorial port #1.
ToFu is a specialised library for tomographic inversion and includes models for various diagnostics such as interferometry, soft and hard X-ray, polarimetry, visible spectrometry, Bremsstrahlung, and bolometry. Fig. 7 shows an example of using ToFu to simulate the signals from ITER bolometers (only the equatorial pinhole camera is shown for illustration). It takes the edge_sources, wall and bolometer IDSs as input and computes the bolometer IDS with the synthetic measurements of brightness or received power on each bolometer.

FIG. 7. Left: Line-of-sight length for the various bolometer channels of equatorial pinhole cameras, displayed in their top view and poloidal view. Right: Resulting brightness for the various bolometer channels.

In the area of visible spectroscopy modelling a new generic CAmera and SPectroscopy Emission Ray-Tracer, CASPER, is being developed. This code provides the raw and first level of analysed data to visible spectrometers and cameras, e.g. the light spectrum, the bremsstrahlung level, and the line intensities etc. The diagnostics models constructed using it, e.g. the Visible Spectroscopy Reference System, Charge Exchange Reference System, H-alpha, and Divertor Impurity Monitor, will individually receive the light spectrum in their appropriate wavelength range to produce the second level of analysed data, which consists of the synthetic signal itself, e.g. the ion temperature, ion rotation velocity, electron density, Z_{eff}, etc. As an illustration, Fig. 8 shows the core and edge profiles used as input to the Visible Spectroscopy Reference System (VSRS), aimed at providing measurements of the line-averaged Z_{eff} and electron density. The inputs are taken from JINTRAC and SOLPS-ITER simulations in the IMAS scenario database and the resulting evaluation of the spectral radiance shows the line emissivities and the bremsstrahlung background evaluation. This model takes the core_profiles, edge_profiles, equilibrium and spectrometer_visible IDSs as input, and delivers the synthetic signals in the spectrometer_visible IDS.

FIG. 8. 2D edge and core profiles taken from SOLPS-ITER and JINTRAC scenarios and resulting spectral radiance including the line emissivities for the various impurities and the bremsstrahlung background level. The green curve shows the realistic case (with a viewing dump limiting the light reflection) and the worst case scenario (with no viewing dump, i.e. with full reflection).

A dedicated diagnostic workflow following a similar concept to the H&CD workflow is under construction to combine all these diagnostic models together and enable synthetic data to be calculated for any diagnostic from any scenario in the IMAS database (as long as the relevant IDSs are present).

9. LIVE DISPLAY

In preparation for the Live Display of information during ITER operations, work has started on the creation of displays using the scenario information contained within the ITER scenario database together with synthetic
diagnostics. Figure 1 shows a still frame of an evolving Live Display derived from data calculated with the METIS [14] and SOLPS-ITER [15] physics codes.

Figure 1. Example control-room Live Display calculated using ITER scenario database and showing plasma equilibrium, waveforms and profiles (based on shot=110005; run=1), together with synthetic views from the Wide Angle Viewing System (WAVS) (based on shot=122264, run=1).

10. SUMMARY AND OUTLOOK

The ITER Integrated Modelling & Analysis Suite (IMAS) has improved its robustness, flexibility and capabilities. Progress has been made towards building a comprehensive High Fidelity Plasma Simulator (HFPS) bringing together state-of-the-art capabilities for the prediction of ITER scenarios, including the sophisticated treatment of plasma heating and current drive elements in a modular manner. Energetic particle stability has been captured in a separate hierarchical approach that can provide analytic estimates all the way up to nonlinear gyro/drift-kinetic numerical calculations. An expanding set of diagnostic models have been implemented and can be used to generate synthetic signals and make diagnostic performance assessments.

*ITER is the Nuclear Facility INB no. 174. The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.*

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