Integrated modelling

The Future of Fusion Energy: Digital Twins and High-Performance Computing

25 September 2024

Kewords

Engineering:

A digital twin is a virtual replica of a physical object, person, or process that can be used to simulate its behavior to better understand how it works in real life.

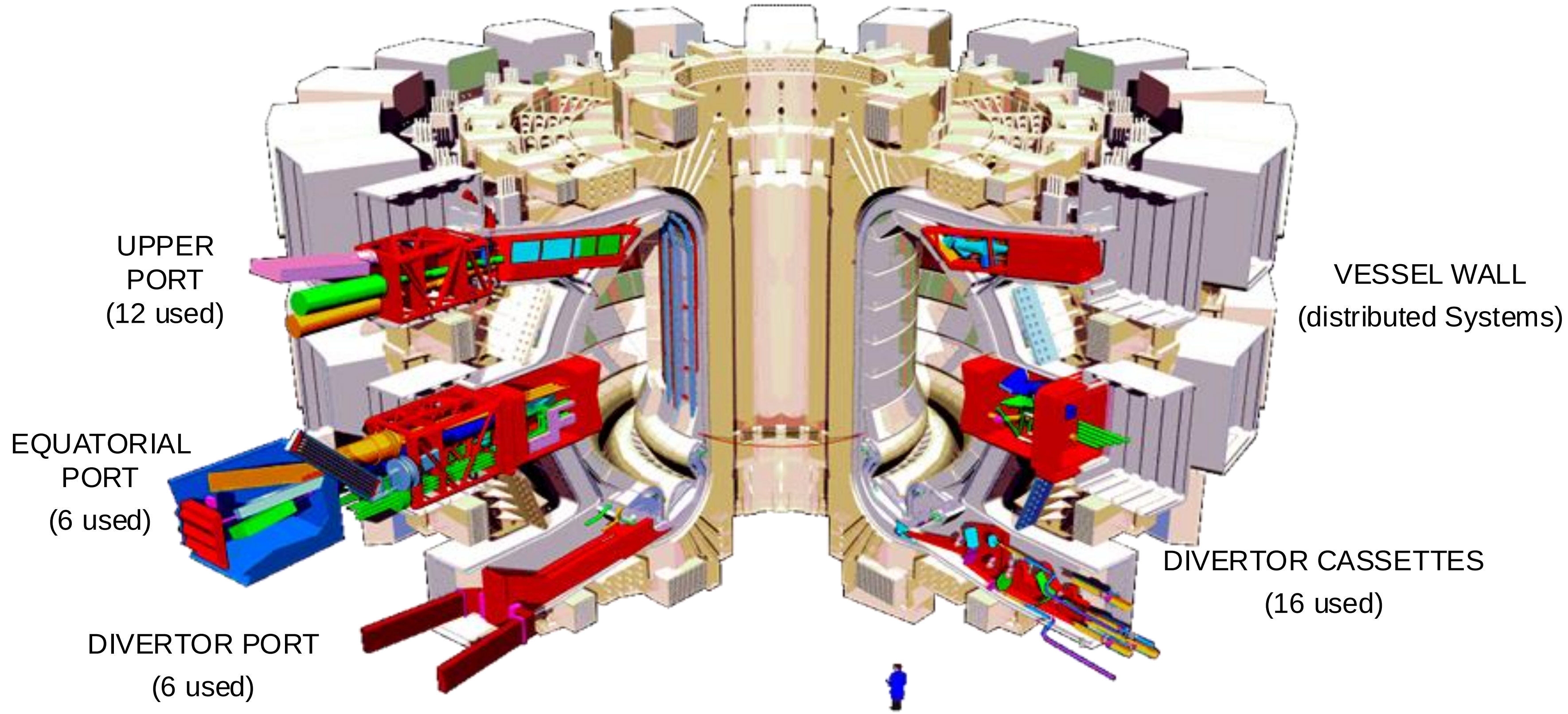
Physics:

Integrated modelling are simulation workflows, incorporating core-edge-SOL/PFC coupling, first-principles models and control elements.

Experimental challenges for analysis (big data)

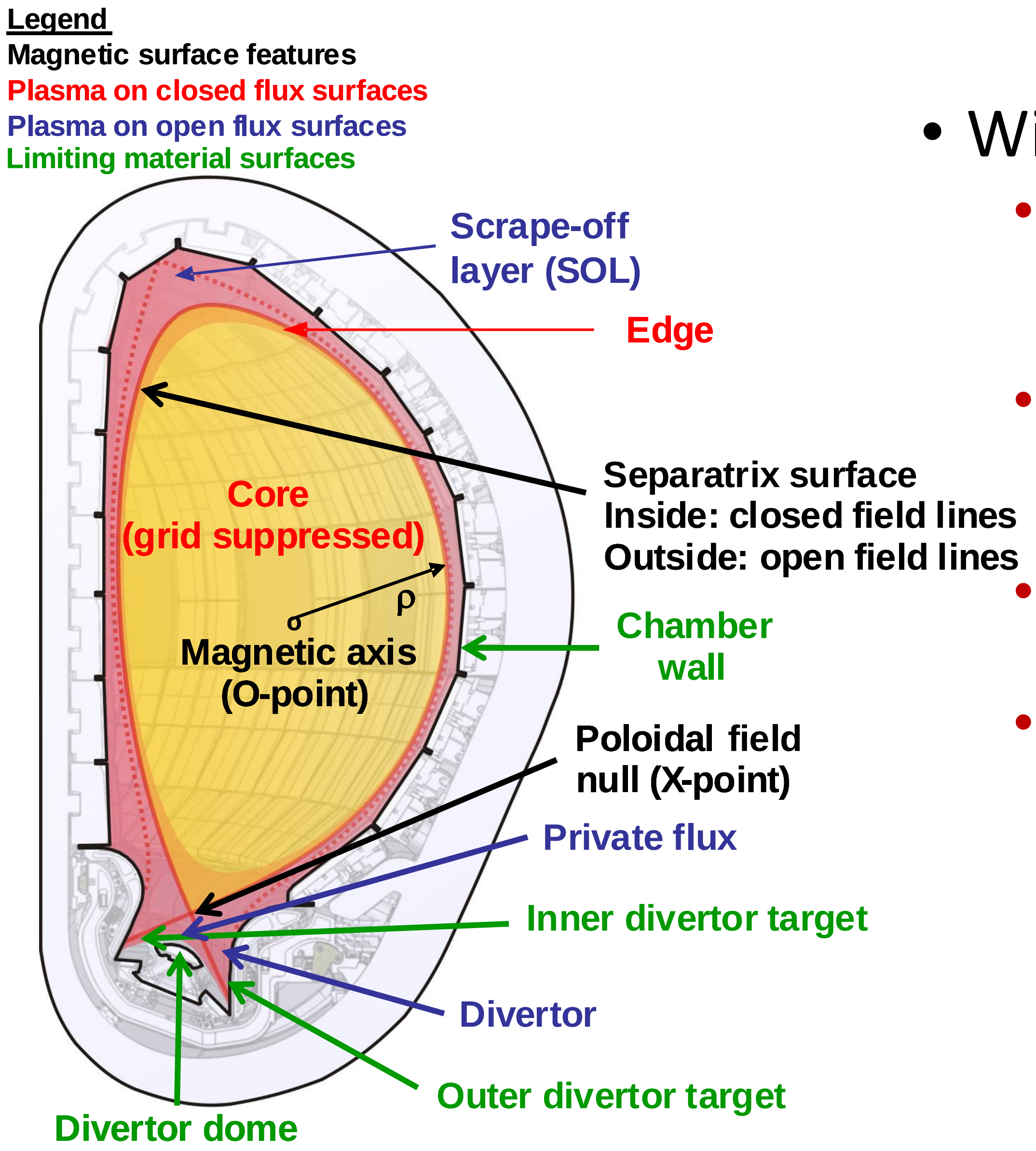
ITER will have around 50 major diagnostic systems

- For machine protection, control and physics studies
- Data volumes expected to reach up to 2.2 PB of raw data per day



Courtesy: S.D. Pinches, ITER

Physics Integration Challenges

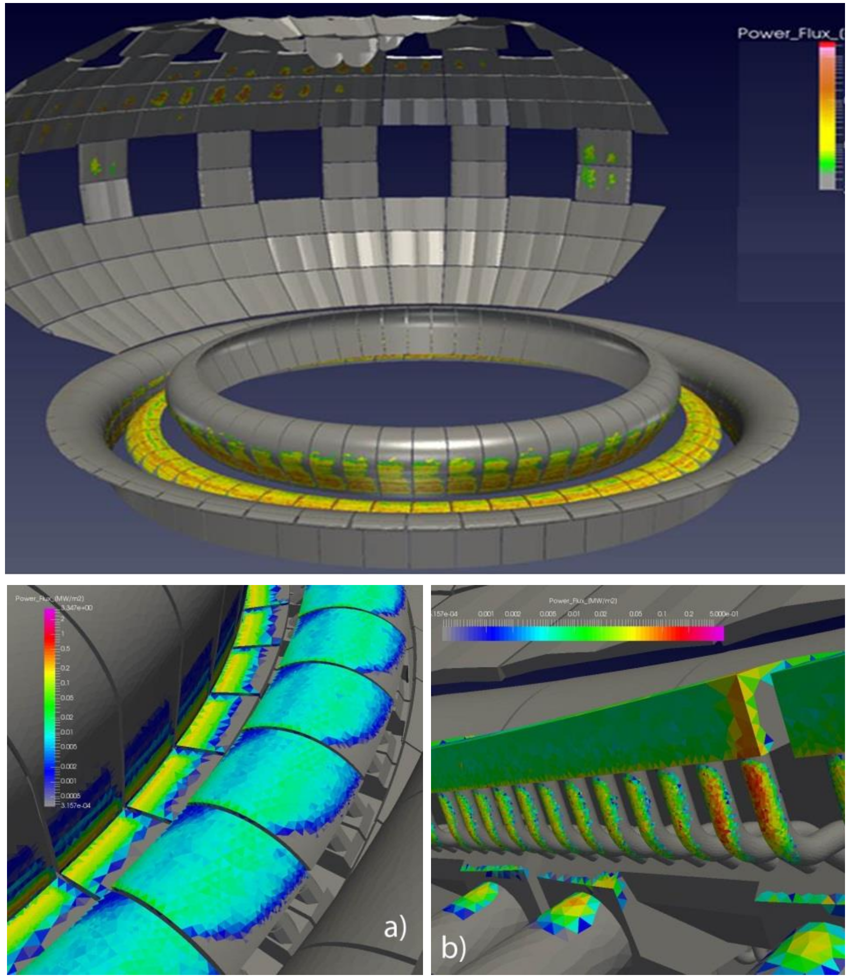


- Will ultimately require:
  - Coupling of all spatial plasma domains (core, edge, scrape-off layer & divertor)
  - Dynamic coupling of individual physics models relevant to each domain
  - Interaction between plasma and plasma facing components
  - Coupling of plasma with external circuits, heating & current drive, fuelling, pumping and other systems to confine and control plasma

Computational Challenges

- Explore new algorithms and techniques as hardware evolves
  - Re-examine traditional approaches
- Exploit advances in architecture
  - E.g. Speed-up ×50 over single core by using GPU to follow fast ions → ×200 using four GPU cards
- Exploit Machine Learning (ML) techniques
  - Speed-up transport models by $\times 10^7$

Beam ion power flux due to 3D fields from ELM coils, TF ripple and ferritic inserts



R. Akers *et al.*, LOCUST-GPU

IMAS

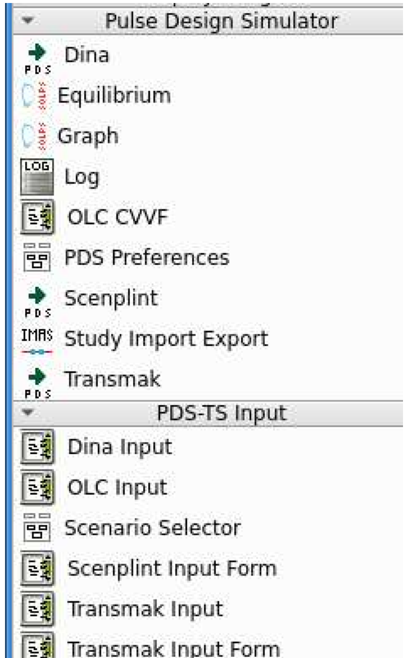
EURO SLING

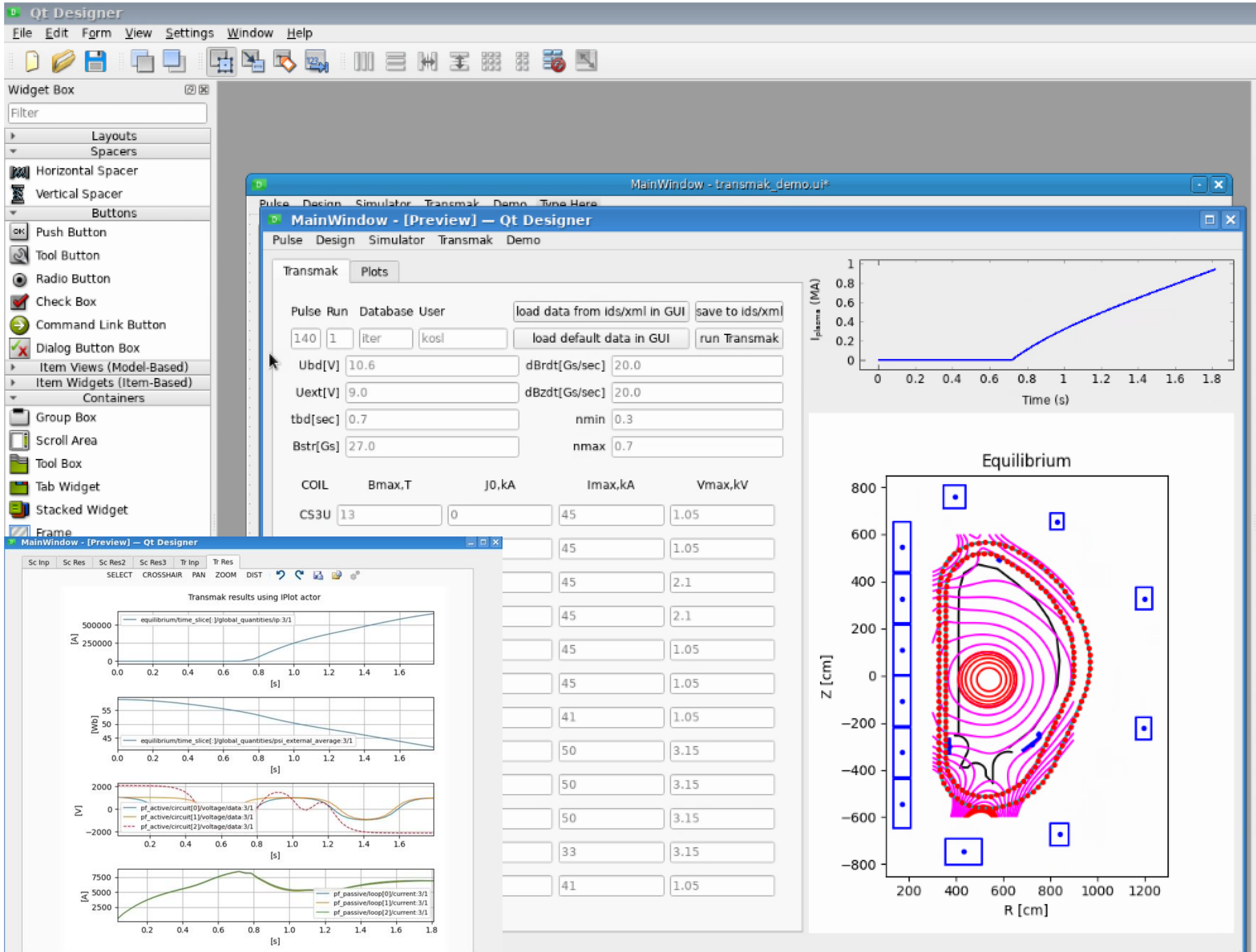
- The Integrated Modelling & Analysis Suite (IMAS) is the collection of software that will be used for all physics modelling and analysis at ITER
- Uses a modular approach that builds around a standardized data representation that can describe both experimental and simulation data for any device
- Inclusion of machine description data allows development and validation of machine-generic components and workflows within ITER Members' programmes before application on ITER

Designing Plasma Simulations with PDS-WF

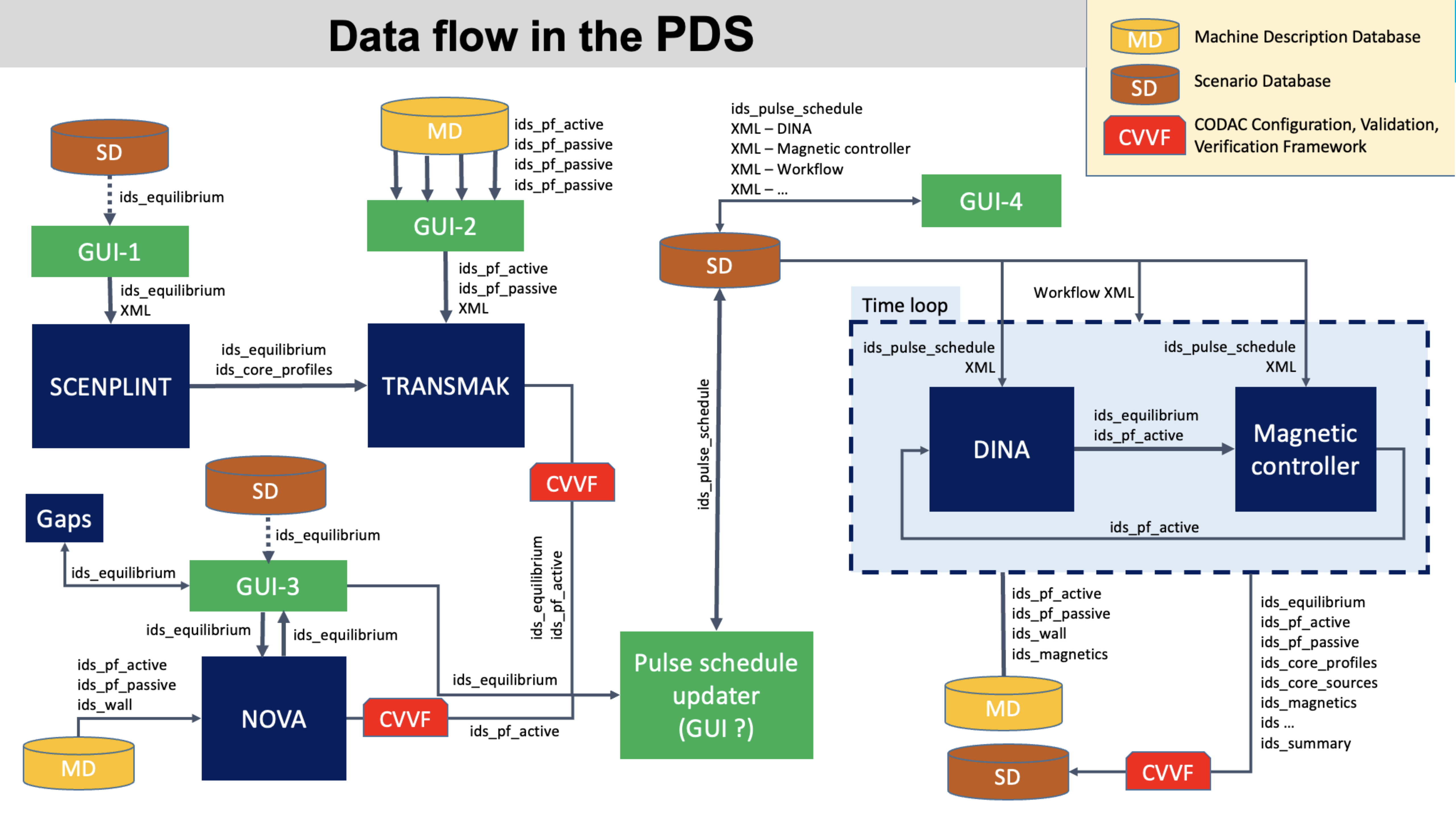
Pulse Design Simulator Workflow is a software environment that we are developing to link codes in the design of first plasma experiments:

- Scenplint
- Transmak
- DINA
- …

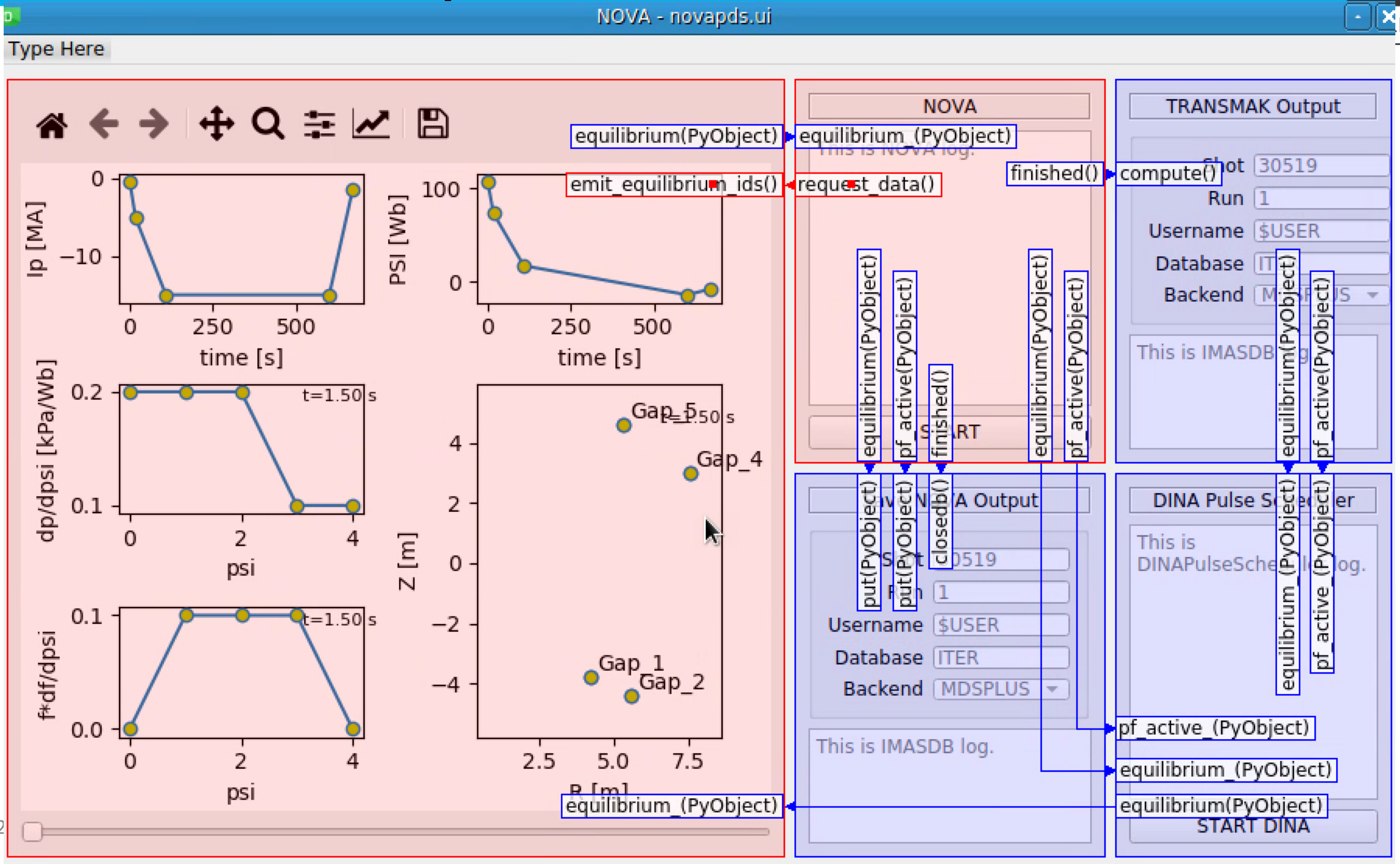




Data flow in the PDS

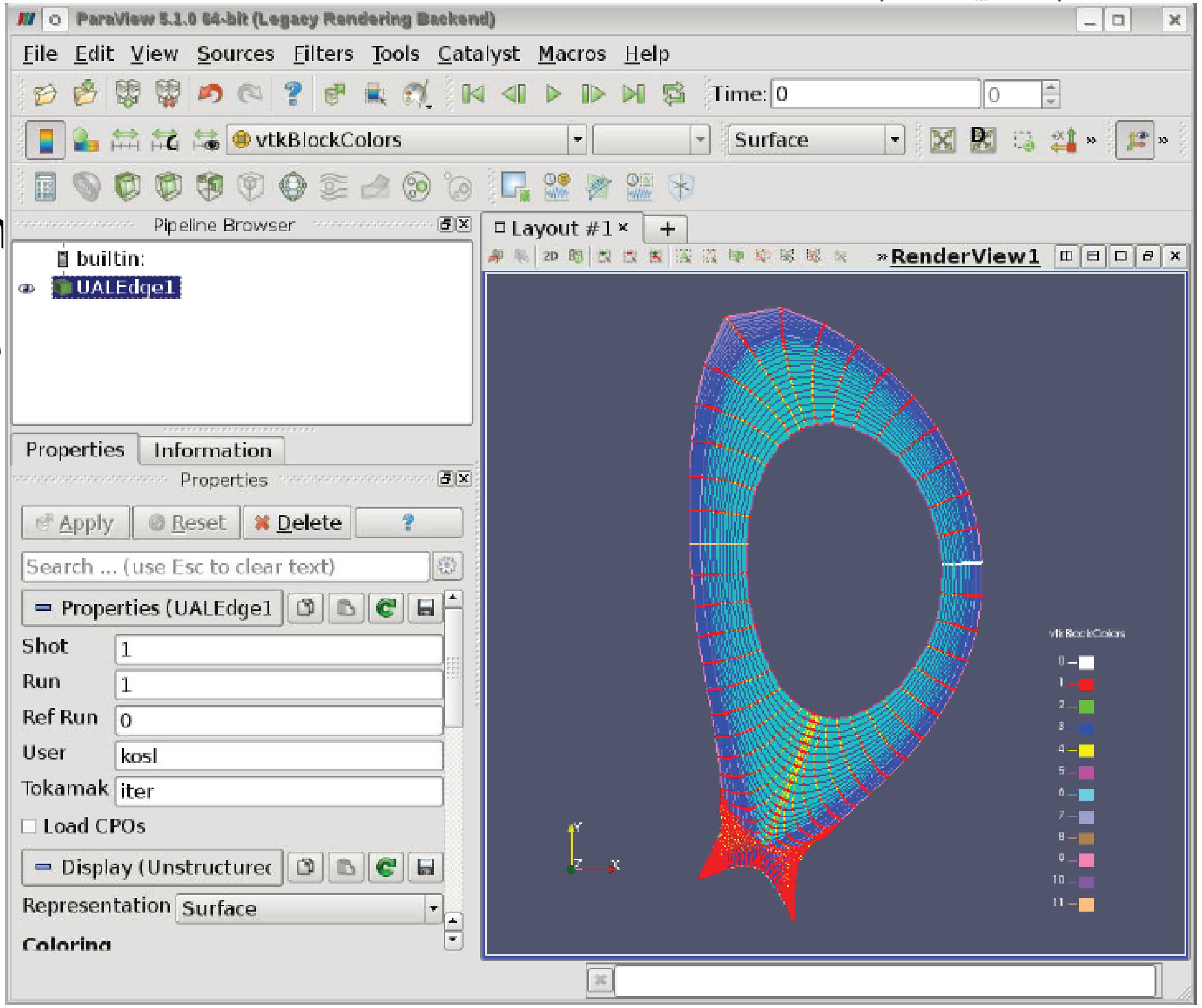


NOVA – DINA pulse schedule workflow



SOLPS-ITER

- SOLPS-ITER is ITER's standard edge physics code
  - Now adapted to archive its data in the form of edge_profiles, edge_sources, edge_transport, and radiation IDSs and use AMNS for A&M rates in B2.5 fluid species
- Now ~500 edge/SOL ITER cases in IMAS database (including all SOLPS4.3 cases)
- New SOLPS-GUI developed to help launch and monitor runs, archive and analyse results in detail
- DivGeo divertor geometry utility can now read/write WALL IDSs



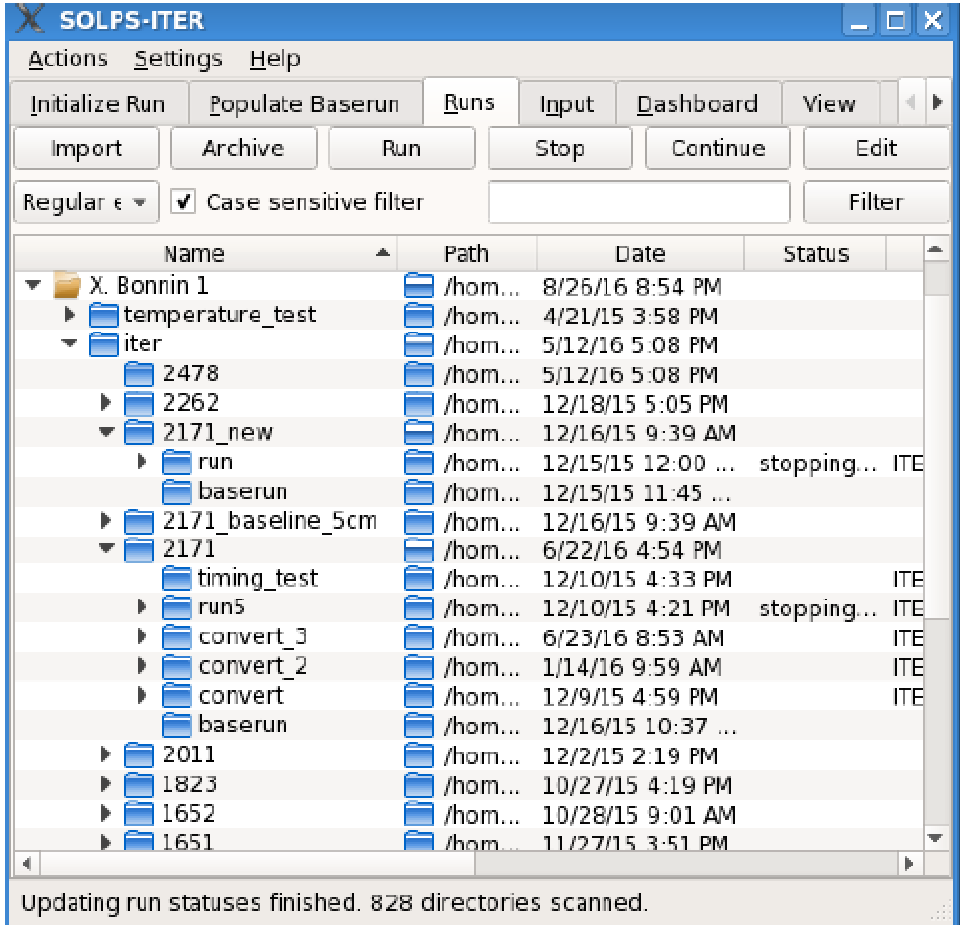
SOLPS-GUI and IMAS support

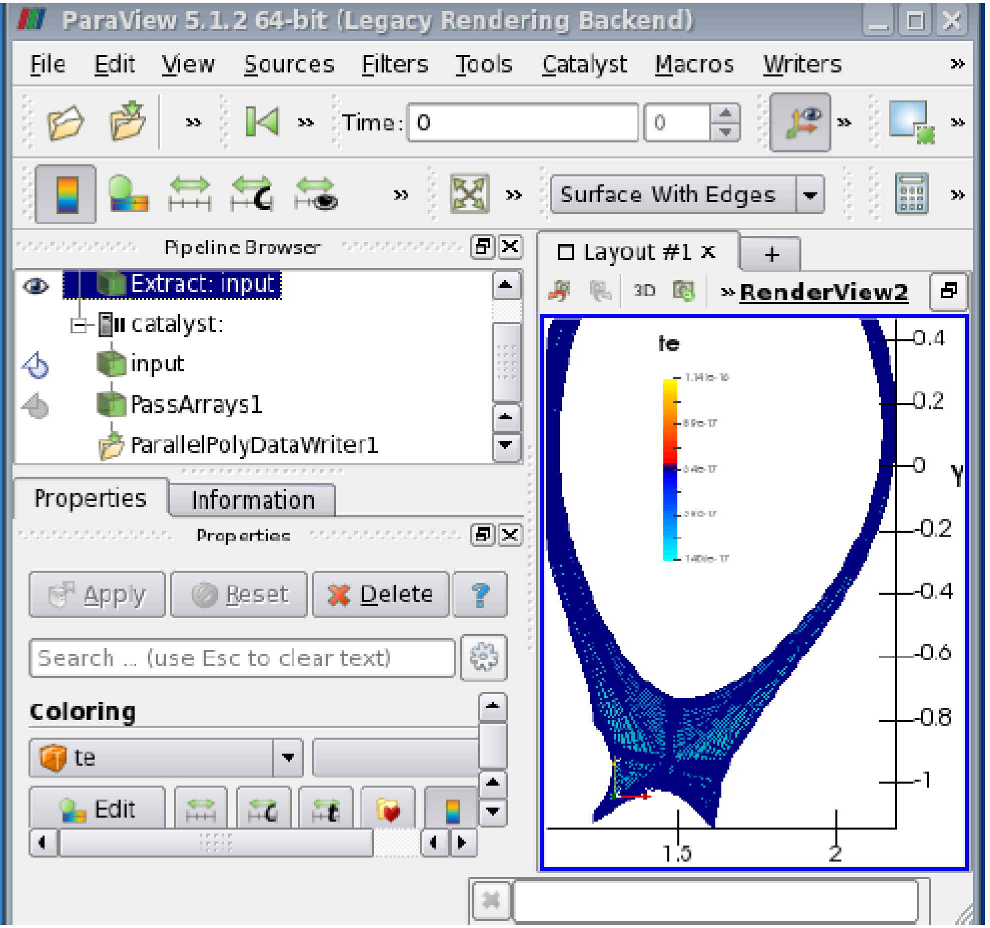
- IMAS: Integrated Modelling Analysis Suite
  - Framework for IM at ITER, distributed to all Members
  - Uses Interface Data Structures (IDSs) to communicate between actors within IM workflows
  - SOLPS-ITER aims to become one such actor
  - CPO2IDS converter tools for backward compatibility with EU-ITM Consistent Physical Objects
  - Archival/retrieval tools with storage of SOLPS runs in IMAS database
- **SOLPS-GUI**:
  - Run monitoring, data display, input builder
  - Inline debugging using Paraview Catalyst
  - Automatic documentation build and cross-referencing using XML and Python tools

HPC Run monitoring and data display

University of Ljubljana
Faculty of Mechanical Engineering

EURO
SLING

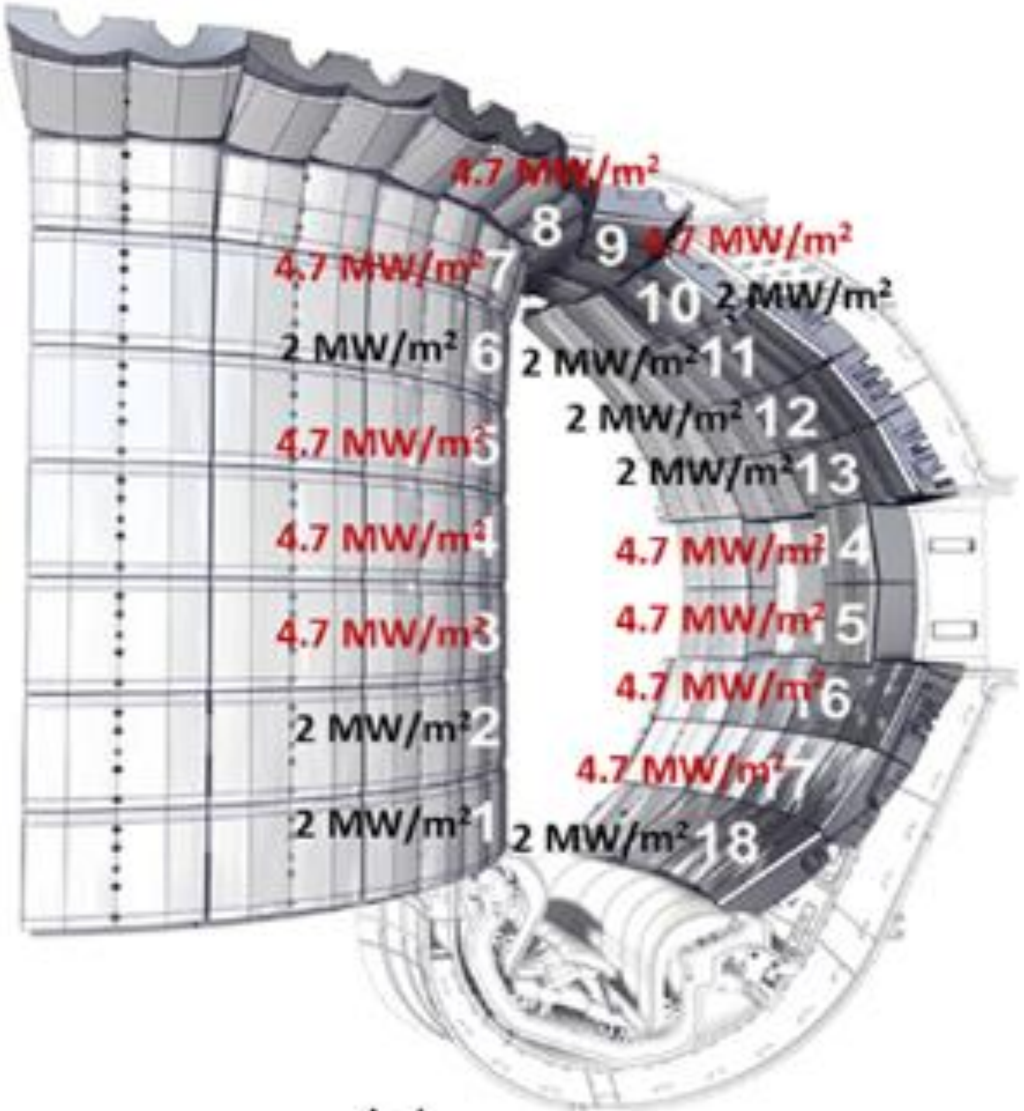




Navigation among run directories

Data display after importing stored solution from **SOLPS-ITER** output files, or IDSs

Plasma Facing Components (PFC)

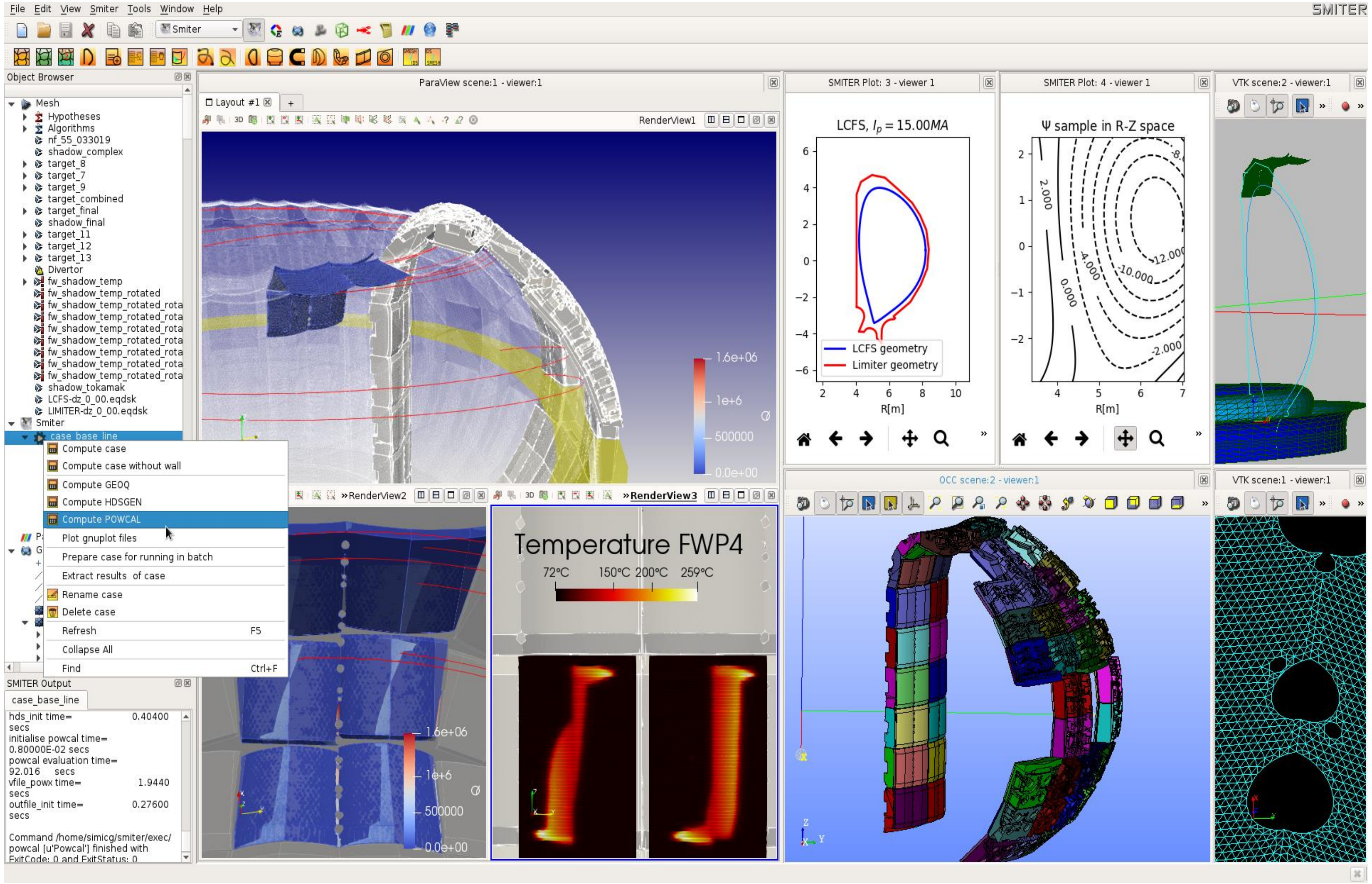


(a)

(b)

SMITER magnetic field-line tracing code

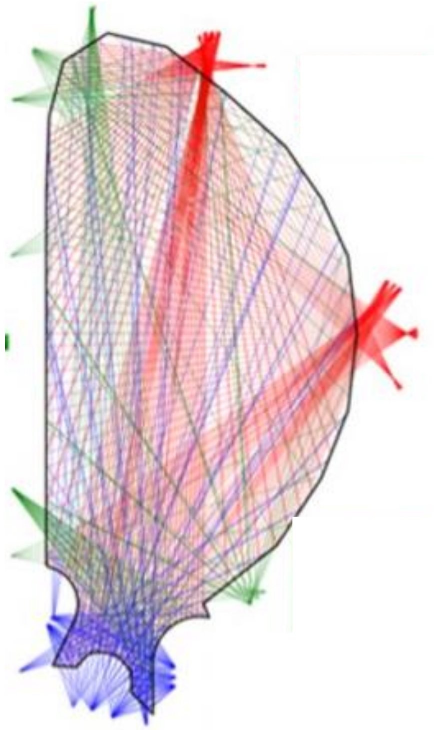
- SMITER addresses a variety of use cases:
  - Power deposition mapping onto first wall and divertor PFCs
  - Input to control algorithms and production of synthetic surface temperatures for diagnostic design
- Can read/write and manipulate WALL and EQUILIBRIUM IDSs
  - Makes extensive use of the IMAS Generalised Grid Description



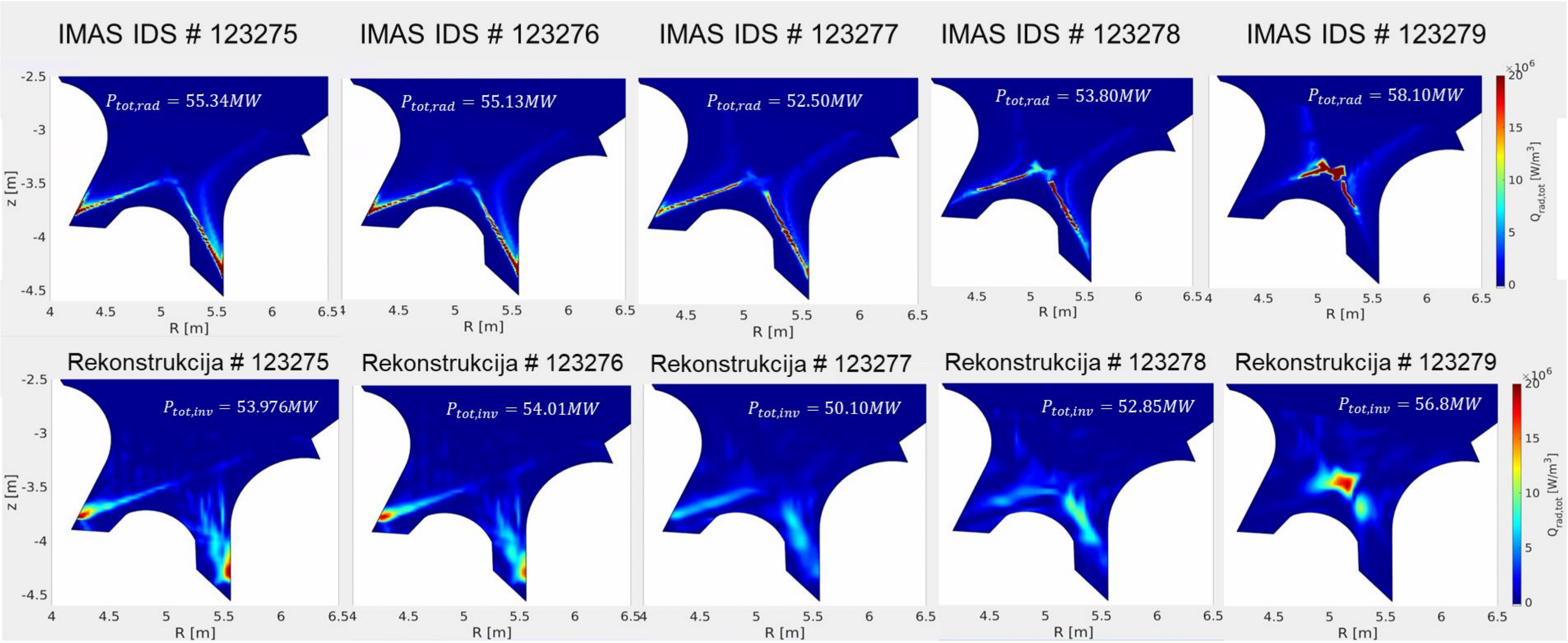
L. Kos *et al* ., Fus. Eng. Des, (2019)

Reconstruction of Plasma Radiation Profiles

Via synthetic bolometer signals
Calculation of synthetic signals on a realistic radiation profile of plasma
Reconstruction of the radiation profile of plasma from synthetic signals (inverse problem)



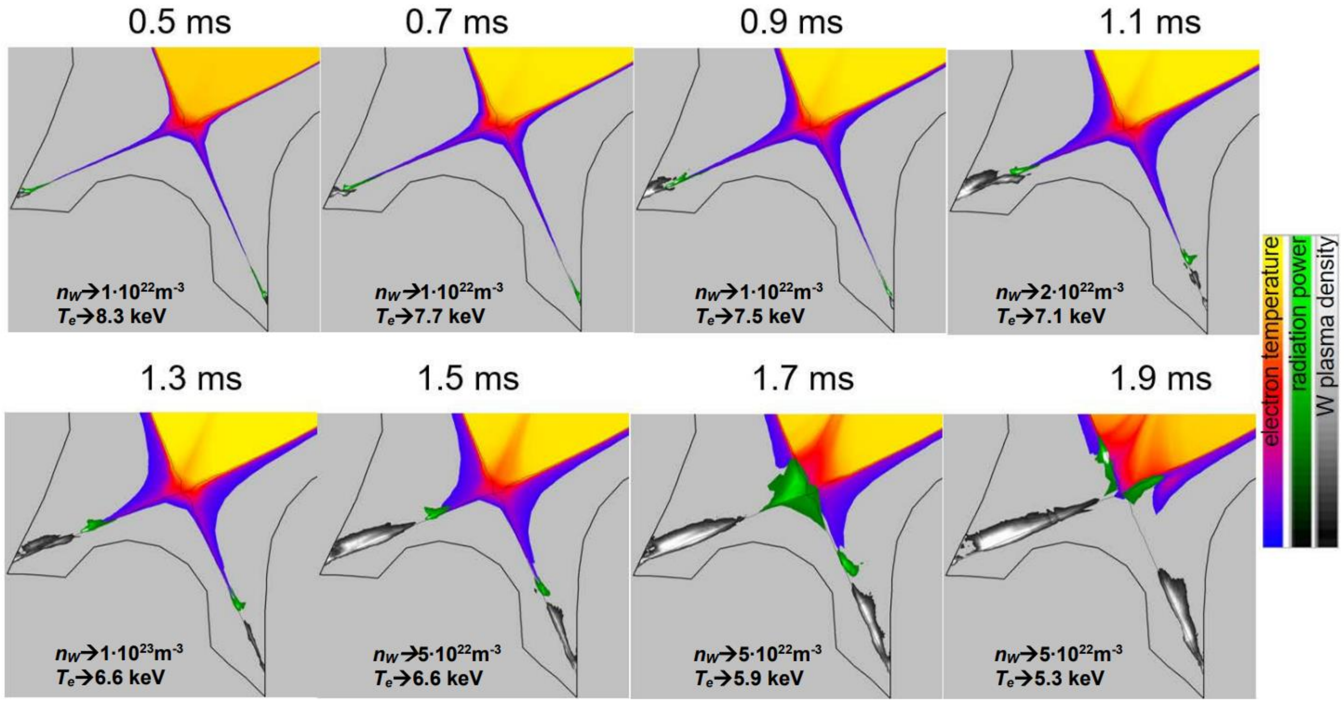
Position and field of view of bolometers, illustrated by a line.



Reconstruction of profiles (below) for 5 realistic SOLPS cases (above), when adding No to the plasma causes the displacement of the maximum radiation fluxes from the reactor wall towards the X-spot (from left to right).

TOKES ("Tokamak Equilibrium and Surfaces")

- The main advantages of the code: fast execution of simulation runs, parametric studies on the reactor scale
- simulation of fast transients of thermal loads PFC (ELM), simulation of SPI and MGI
- computation of multifluidic processes (including impurities and neutral flows) in nuclear and SOL plasmas
- Standard surface interactions: "sputtering", simulation of surface evaporation and vapor shield...



TOKES simulation of uncontrolled disturbance of the initial plasma energy 280 MJ

- JOREK is a code developed by several laboratories
- solve nonlinear MHD equations in reduced or full form, including toroidal corrections,
- The code simulate with a full-f particle-in-cell scheme
- It can use several models to simulate X-point plasma with realistic physics
- Spatial discretization is made through third order Bezier finite elements, and the time integration are carried out fully implicitly.
- It couples the computation of kinetic Boltzmann equations to MHD fluid with its space-and time-discretization.
- The code uses local coordinate in the spatial discretization, with the radial component and the angular component, on a poloidal cut of the torus.
- It can take anisotropic distribution of energetic particles for simulations.
- Radiation, recombination and ionization model are included. It contains a kinetic module, modeling a broad range of particles, up to relativistic speed for the electrons.
- For viability, the code have been benchmarked against other MHD codes and the discharges from ASDEX-Upgrade.
- To compute faster, JOREK uses a hybrid OpenMP/MPI system, with MPI tasks and OpenMP threads being run on the Marconi-Cineca HPC server.

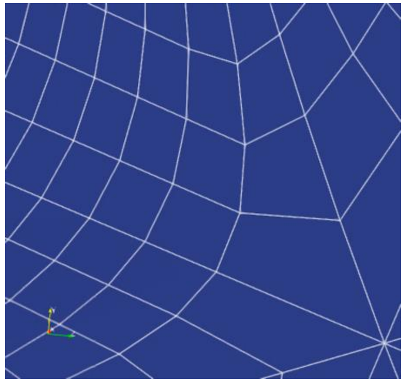
Visualisation of MHD IDS

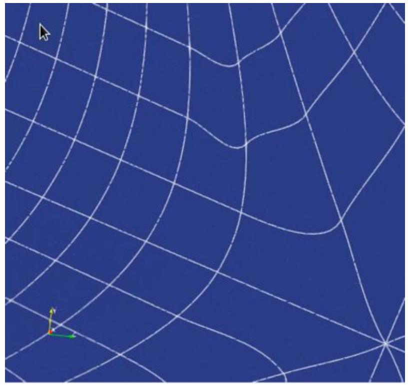
From:

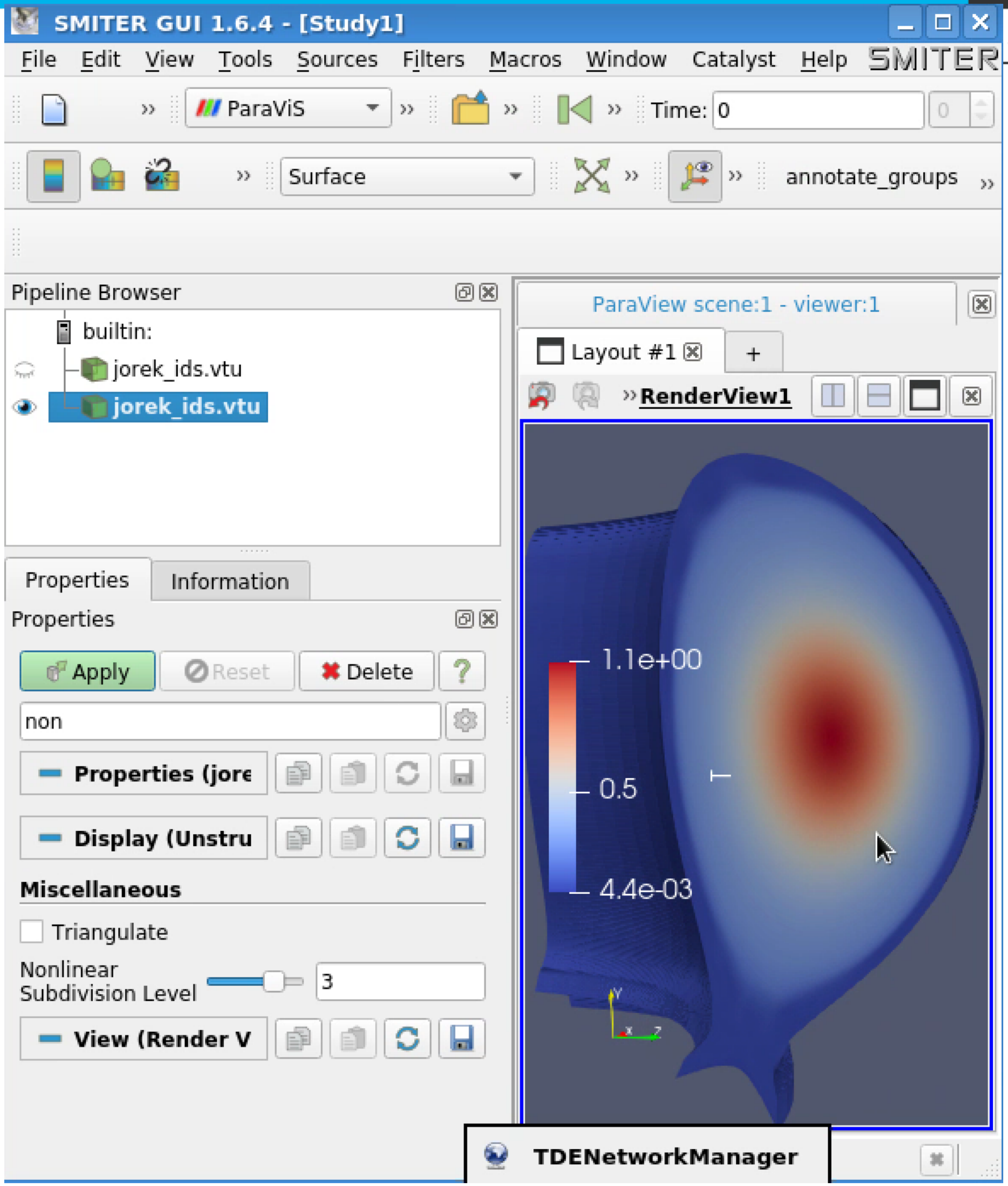
- VTK 9.0
- ParaView 5.9.1
- SMITER/1.6.3+

- Nonlienar subdivision

non=0 non=3

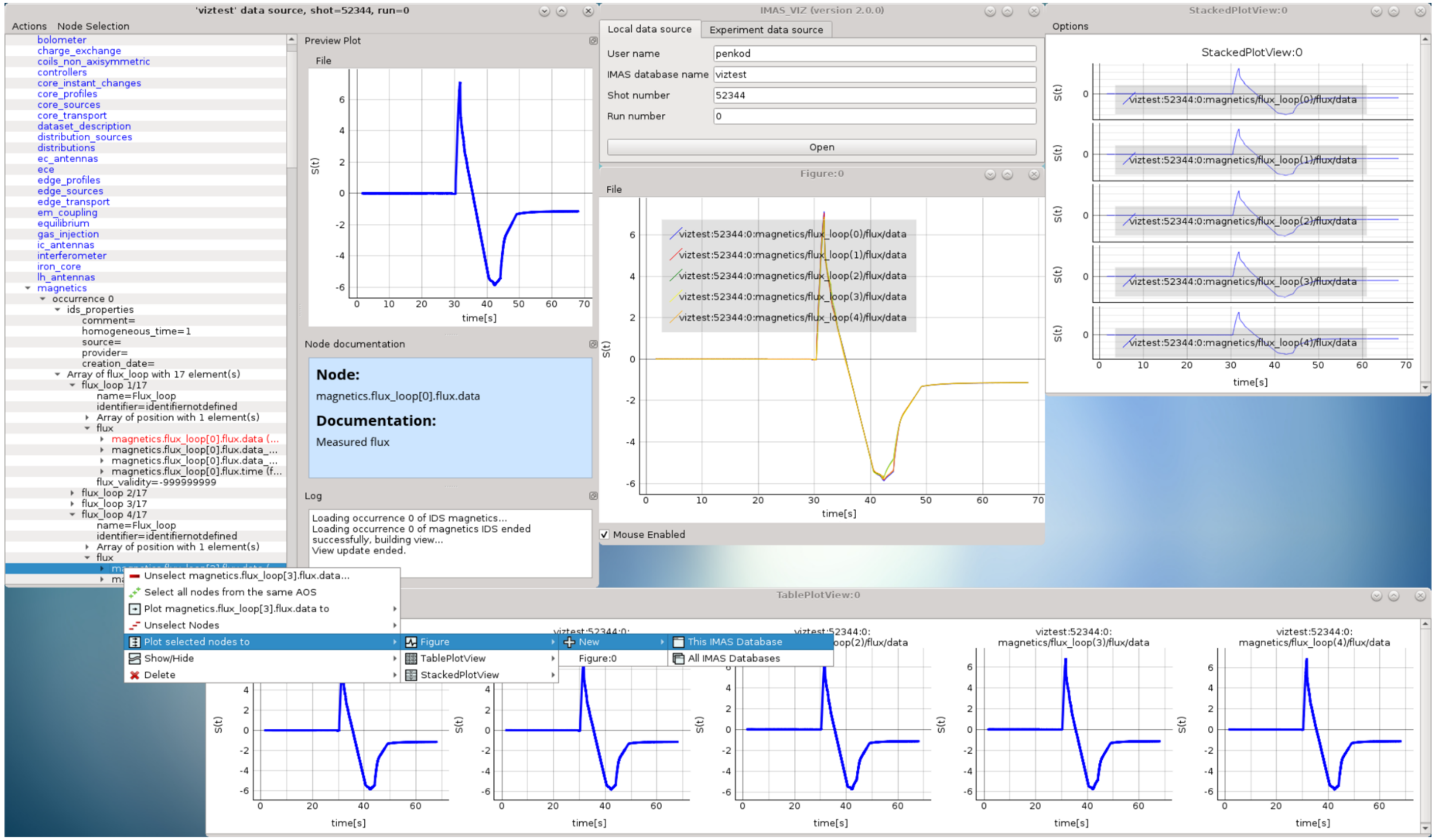






IMASViz

IMASViz is a visualization tool developed used within Integrated Modelling Analysis Suite (IMAS) for the purposes of visualizing static and dynamic IMAS data, stored within IMAS Interface Data Structures (IDSs).



Outline of ITER's IM and Analysis Needs

- Predictive workflows for simulations of ITER operation
  - Complete pulse from breakdown to termination
  - Respecting plant limitations (e.g. PF circuits)
  - Free-boundary magnetic equilibrium evolution including realistic plasma transport
    - With multiple impurities (W, Be, He, Ne, Ar, N,…)
  - Extensible to include the plasma edge, scrape-off layer (SOL) & plasma facing components (PFCs)
  - Modular inclusion of sources: heating & current drive (H&CD), fuelling (pellets & gas)
  - Description of transients: confinement (L-H), instabilities (e.g. MHD)
- Hierarchy of validated physics models and workflows of varying degrees of physics fidelity and computational performance
  - Scenario development and physics validation tools including interface with Plasma Control System Simulation Platform (PCSSP)

Outline of ITER’s IM and Analysis Needs

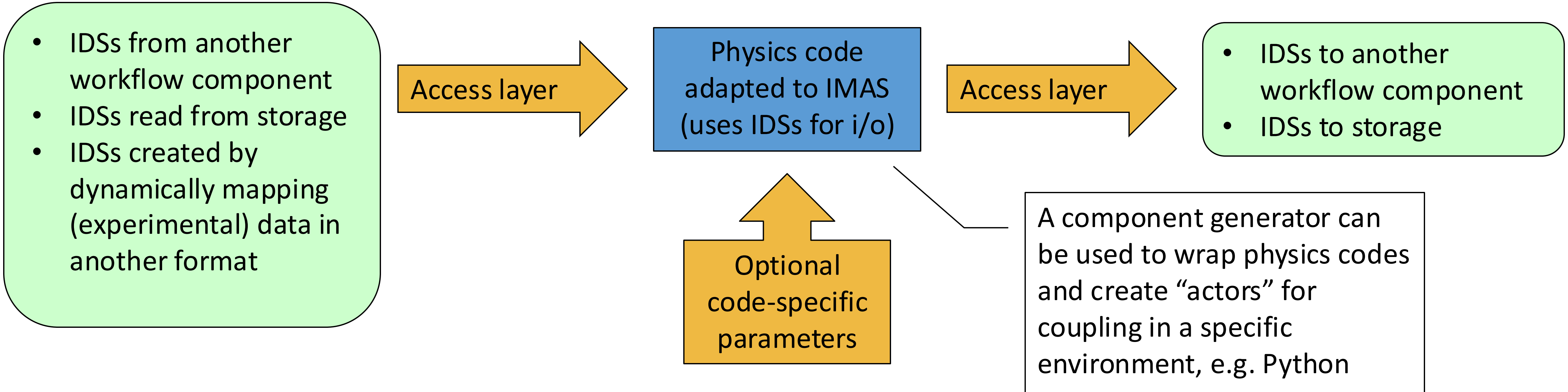
- Analysis, data processing and visualisation tools
  - Hierarchy of plasma reconstruction chains: magnetics-only equilibrium reconstruction → interpretive transport simulations
  - Inference capability to determine physics parameters and their uncertainties from raw measurements
    - Flow-down of diagnostic signals to meet Project Measurement Requirements
    - Diagnostic models (synthetic diagnostics) to support design and performance assessments
  - Data visualisation tools capable of supporting Operations (including Live Display) and Research
  - Tools to support data discovery and listing/filtering data by given criteria

Data Model

- Data Dictionary defines structuring and naming of data
  - Same data structures used for both experimental (all devices) and simulation data
  - Applicable to all devices (includes Machine Description data) – not restricted to ITER
  - Precise design rules ensure global homogeneity
  - Uses a tree structure (allows re-use of names)
  - Well-defined lifecycle procedures allow collaborative evolution of Data Model
- Interface Data Structures (IDSs)
  - Standardised entities for use between software components and storage
    - Examples include plant systems (*diagnostics, heating systems*) and physics concepts (*equilibrium, core plasma profiles*)
  - Contains traceability (provenance) and self-description information
  - Supports modularity and facilitates interchange of components from contributors

Using Interface Data Structures (IDS) to couple codes

- The IMAS Access Layer is used to retrieve/store data and also makes coupling codes using IDSs straightforward, even if they are written in different languages
  - Automated definition of data structures for all supported languages
  - Fortran, C++, Python, Java, MATLAB
- This is the basis upon which modular workflows such as plasma simulators and data processing chains are created



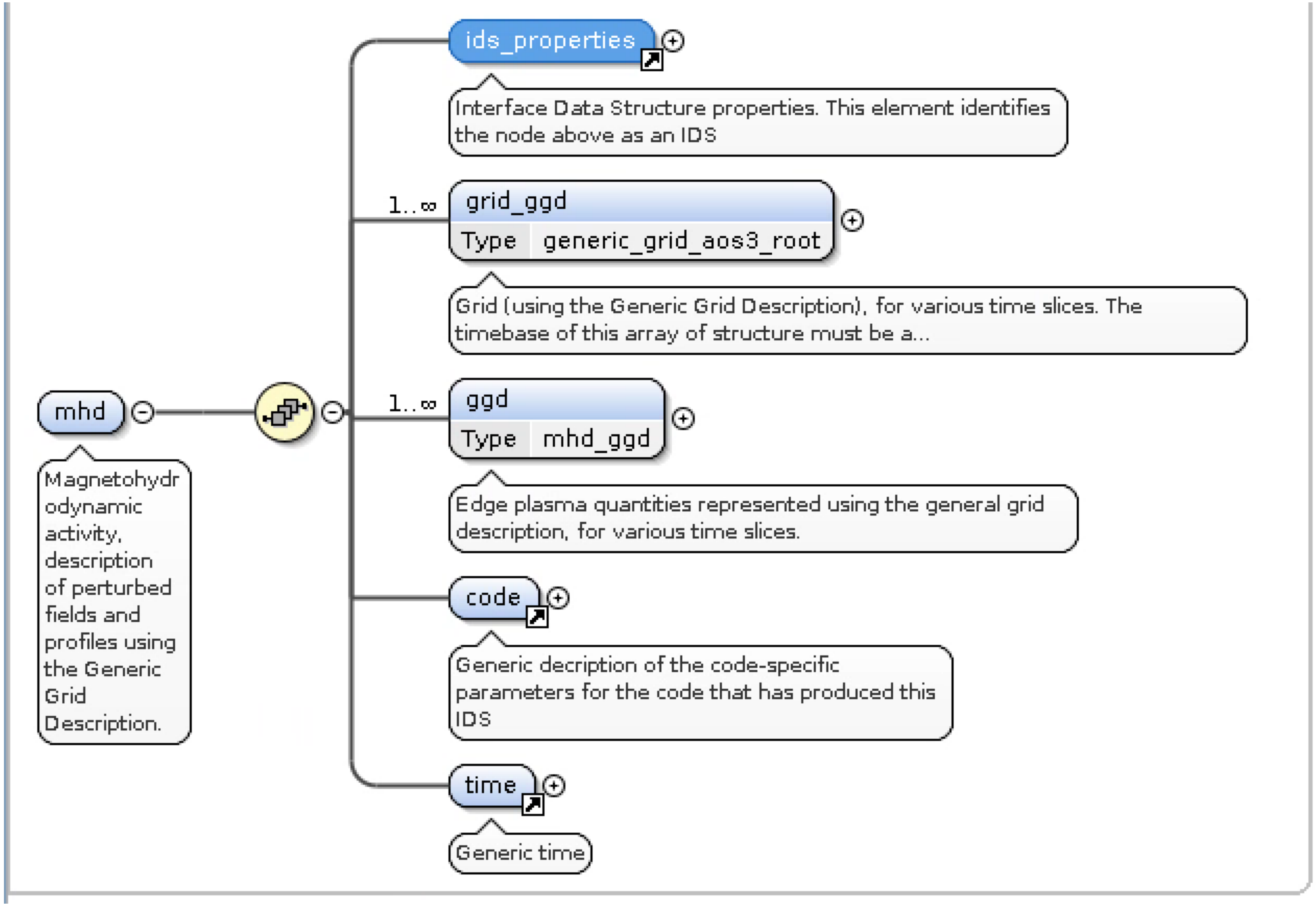
IMAS Data Model

Heating systems | Diagnostics

amns_data	disruption	iron_core	reflectometer_profile
barometry	distribution_sources	langmuir_probes	refractometer
bolometer	distributions	lh_antennas	sawteeth
bremsstrahlung_visible	divertors	magnetics	soft_x_rays
calorimetry	ec_launchers	mhd	spectrometer_mass
camera_ir	ece	mhd_linear	spectrometer_uv
camera_visible	edge_profiles	mse	spectrometer_visible
charge_exchange	edge_sources	nbi	spectrometer_x_ray_crystal
coils_non_axisymmetric	edge_transport	neutron_diagnostic	summary
controllers	em_coupling	ntms	temporary
core_instant_changes	equilibrium	pellets	thomson_scattering
core_profiles	gas_injection	pf_active	tf
core_sources	gas_pumping	pf_passive	transport_solver_numerics
core_transport	gyrokinetics	polarimeter	turbulence
cyrostat	hard_x_rays	pulse_schedule	wall
dataset_description	ic_antennas	radiation	waves
dataset_fair	interferometer	real_time_data	workflow

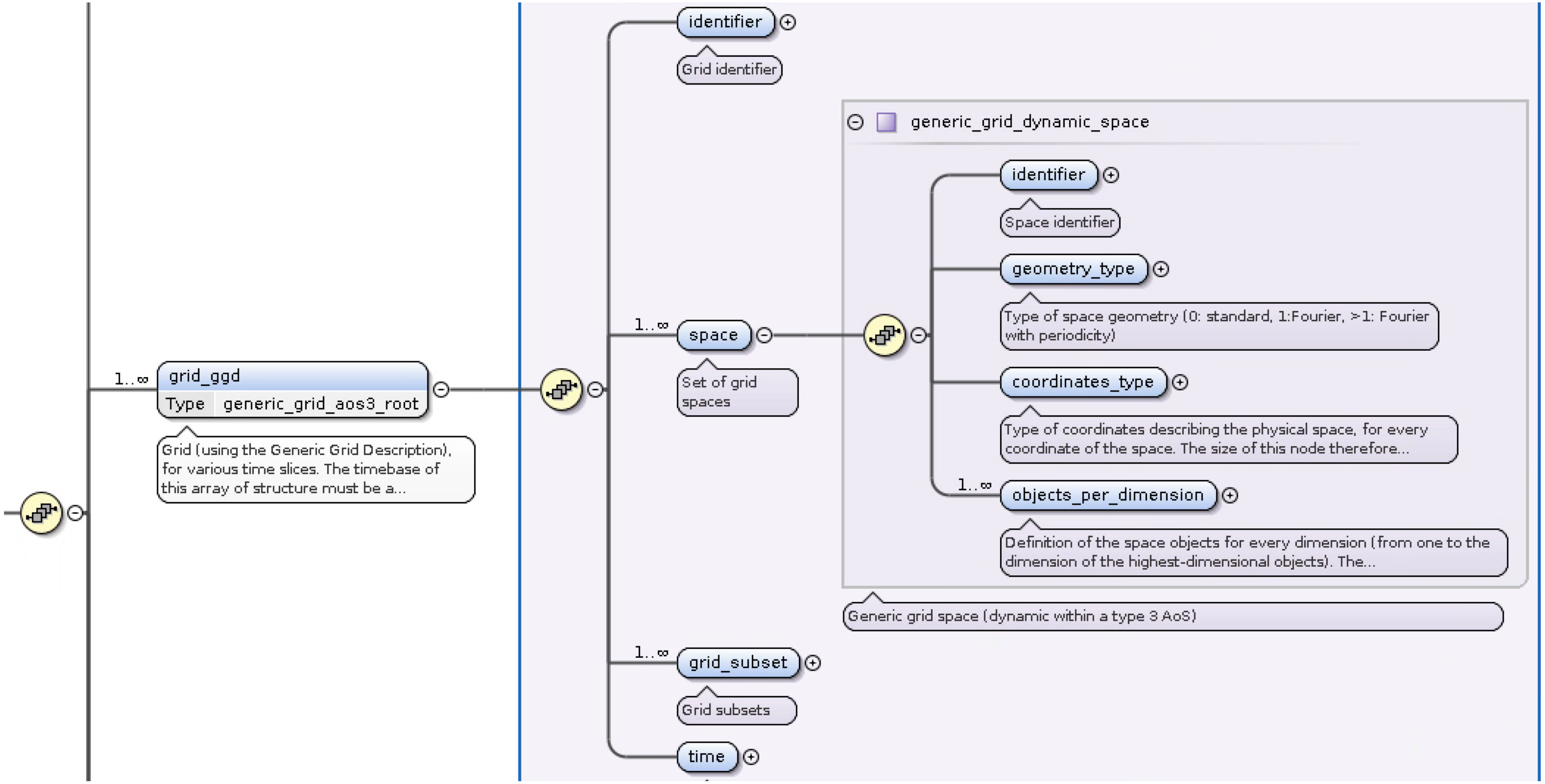
Extension of Data Dictionary mainly through application to new Use Cases and user feedback. For more details, see links from https://imas.iter.org.

IMAS MHD Interface Data Structure



General Grid Desrciption (GGD)

- Grid GGD (grid_ggd) describes the grid geometry

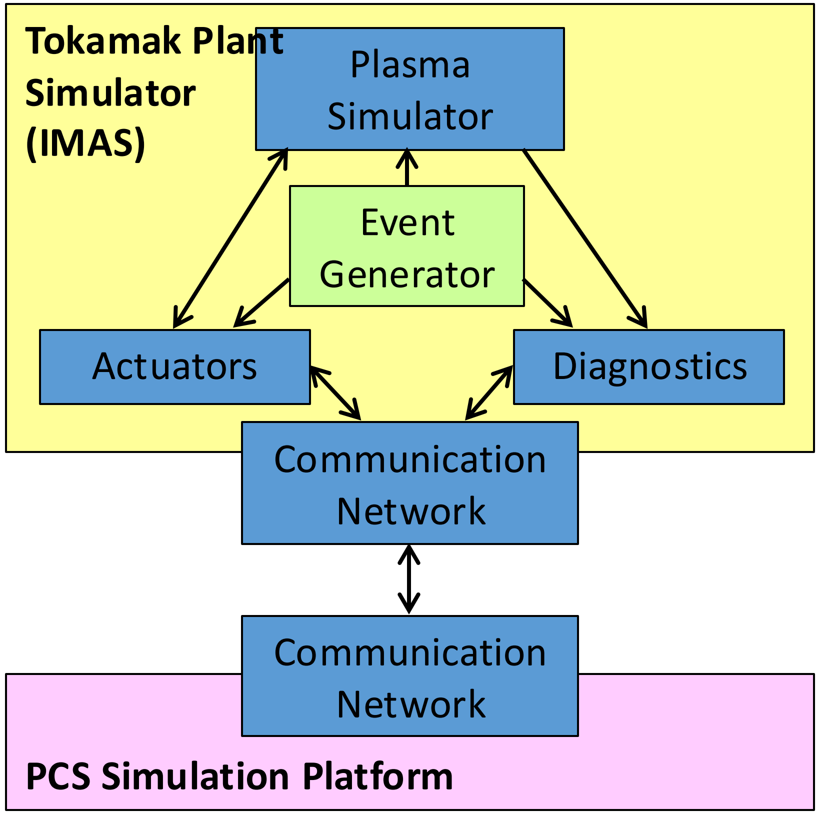


Validating IMAS Components and Workflows

- Validation is an important element of IMAS development
- Validation needs data
- Data is only available on existing machines
  - IMAS needs to connect to existing (as well as future) data
- Existing experimental data stored in wide variety of formats
  - ITER DAN data will be stored as HDF5
- IMAS needs to be able to read different storage formats and map into IDSs
  - Data owners write (UDA) plug-ins to read their data formats and map into Data Model
  - On-going voluntary activity with Members
- Mapping device-specific data into Data Model needs managing
  - Data Model allowed to evolve (latest release is v3.34.0)
  - Plug-in based technology demonstrated to manage mapping (e.g. by shot ranges)

IMAS Plasma Simulator

- One of the principle deliverables from the IMAS programme is a plasma simulator to support physics validation of plasma scenarios
- Co-simulations of Plasma Simulator and Plasma Control System Simulation Platform (PCSSP)
  - Basis for physics validation
  - Develop control strategies from plasma initiation to burn control
  - Refine response to events
    - L-H transition
    - Power supply interruption
    - Diagnostic degradation / failure



Ingredients of High-Fidelity Plasma Simulator

- IO doesn't have resources to develop a full plasma simulator from scratch
- Many existing plasma simulators with a long history of refinement and exploitation have been used by the IO to support the ITER design and the development of the ITER Research Plan, including
  - ASTRA, CORSICA, DINA, JINTRAC, TRANSP,…
- Following initial efforts to align on-going voluntary efforts with IMAS, we now focus upon integrating and refactoring the following key components
  - JINTRAC for core-edge coupled transport simulations (particles and energy)
  - DINA for evolution of magnetic equilibrium and poloidal field (PF) circuit
- In addition, IO staff and interns have developed a Heating & Current Drive (H&CD) workflow to describe (synergistically) all the ITER plasma heating systems and provide the source terms for a HFPS transport solver

- Machine Description available for H&CD systems, many diagnostics, wall, magnetics and coils

IMAS Machine Description databa

```
[pinches@sdcc-login03 ~]$ md_summary
----> Default call equivalent to:
      md_summary -c pbs,ids,description
---------------------------------------------------------------------------------------------------------------------------------------------
PBS           IDS                         DESCRIPTION                                                                      SHOT/RUN
---------------------------------------------------------------------------------------------------------------------------------------------
PBS-11        pf_active                   PF/CS Coil System, TF busbars (equivalent) and Virtual Coils                     111001/3
PBS-11        tf                          TF Coil System                                                                   111002/1
PBS-11        coils_non_axisymmetric      Ex-Vessel Coils (EVC) Systems (CC)                                               111003/1
PBS-15        coils_non_axisymmetric      In-Vessel Coils (IVC) Systems (ELM)                                              115001/1
PBS-15        coils_non_axisymmetric      In-Vessel Coils (IVC) Systems (ELM periodic)                                     115002/1
PBS-15        coils_non_axisymmetric      In-Vessel Coils (IVC) Systems (VS)                                               115003/1
PBS-15        pf_passive                  Vacuum Vessel (VV), Triangular Support (TS) and Divertor Inboard Rails (DIR) from IDM  115004/1
PBS-15        pf_passive                  Vacuum Vessel (VV), Triangular Support (TS) and Divertor Inboard Rails (DIR) from DINA 115005/2
PBS-55.D1     bolometer                   PP pinholes and collim., Div. collim., VV collim. (550 channels)                 150401/2
PBS-55.E5     spectrometer_x_ray_crystal  Core X-Ray Spectrometer (XRCS)                                                   150505/2
PBS-55.EC     spectrometer_visible        Charge Exchange Recombination Spectroscopy (CXRS) Edge                           150512/2
PBS-55.E1     spectrometer_visible        Charge Exchange Recombination Spectroscopy (CXRS) Core                           150501/2
PBS-55.EF     spectrometer_visible        Charge Exchange Recombination Spectroscopy (CXRS) Pedestal                       150515/2
PBS-52        ec_launchers                Electron Cyclotron (EC) launchers                                                120000/1
PBS-55.F1     ece                         Electron Cyclotron Emission (ECE) - Radial O-mode                                150601/1
PBS-55.F1     ece                         Electron Cyclotron Emission (ECE) - Radial X-mode                                150601/2
PBS-55.F1     ece                         Electron Cyclotron Emission (ECE) - Oblique O-mode                               150601/3
PBS-55.F1     ece                         Electron Cyclotron Emission (ECE) - Oblique X-mode                               150601/4
PBS-51        ic_antennas                 Ion Cyclotron (IC) antennas                                                      110000/1
PBS-55.C5     interferometer              Toroidal Interfero-Polarimeter (TIP)                                             150305/1
PBS-55.FA     interferometer              Density Interfero-Polarimeter (DIP)                                              150610/1
PBS-55.A*     magnetics                   AD,AE,AF,AH,AI,A3,A4,A5,A6,AA,AB,AJ,AL,A9,AC,AG,AP magnetic systems              150100/3
PBS-53        nbi                         Heating Neutral Beams (HNB) - H beams 870 keV - off-off                          130000/1201
PBS-53        nbi                         Heating Neutral Beams (HNB) - H beams 870 keV - off-on                           130000/1301
PBS-53        nbi                         Heating Neutral Beams (HNB) - H beams 870 keV - on-on                            130000/1501
PBS-53        nbi                         Heating Neutral Beams (HNB) - D beams 1 MeV - off-off                            130000/2201
PBS-53        nbi                         Heating Neutral Beams (HNB) - D beams 1 MeV - off-on                             130000/2301
PBS-53        nbi                         Heating Neutral Beams (HNB) - D beams 1 MeV - on-on                              130000/2501
PBS-53        nbi                         Diagnostic Neutral Beam (DNB) - on-axis                                          130000/3201
PBS-53        nbi                         Diagnostic Neutral Beam (DNB) - off-axis                                         130000/3101
PBS-55.C6     polarimeter                 Poloidal Polarimeter (POP)                                                       150306/1
PBS-55.F9.40  refractometer               Sub-system refractometer of HFS reflectometer                                    150609/401
PBS-55.E6     spectrometer_visible        Visible Spectroscopy Reference System (VSRS)                                     150506/2
PBS-16        wall                        First wall and divertor geometry for PFPO and FPO phases                         116000/2
PBS-16.FC     wall                        First Plasma Protection Components (FPPC)                                        116612/1
PBS-16        pf_passive                  Blanket Module Panel (BMP)                                                       116001/1
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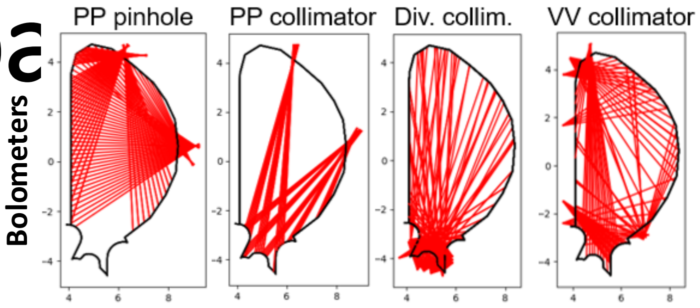
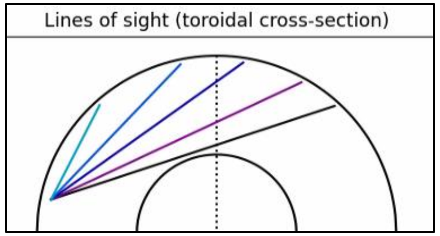
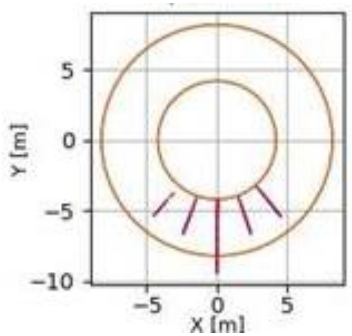
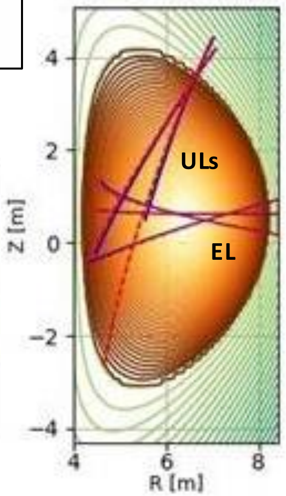


Toroidal Interfero-Polarimeter



EC launchers

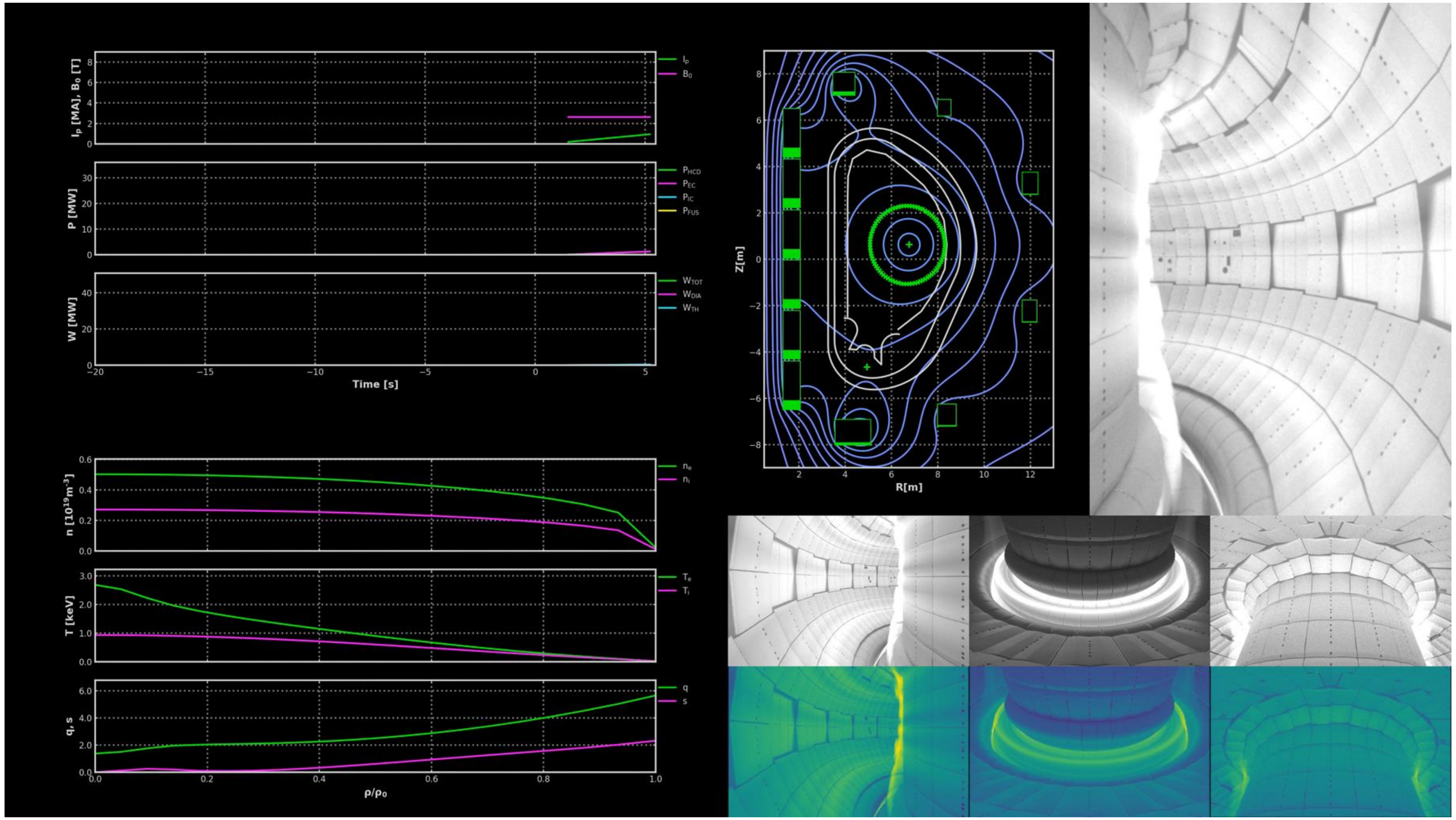




- The MD database provides the geometry of the plant systems to be used as input of simulation codes

Live Display as in Control Room

- Simulation of 7.5 MA / 2.65 T He4 plasma in ITER PFPO



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

Example (Python) script

```
import os, imas
from imas.imasdef import MDSPLUS_BACKEND,CLOSEST_SAMPLE
from dip_tip.wrapper import dip_tip_actor as dip_tip

# SCENARIO AND MD INPUT DATA, LOCAL OUTPUT DATA
shot_scen, run_scen, user_scen, database_scen = 134174, 117, 'public',          'iter'
shot_md,   run_md,   user_md,   database_md   = 150305, 1,   'public',          'ITER_MD'
shot_out,  run_out,  user_out,  database_out  = 134174, 118,  os.getenv('USER'), 'iter'

# OPEN SCENARIO DATA
scenario = imas.DBEntry(MDSPLUS_BACKEND,database_scen,shot_scen,run_scen,user_scen)
scenario.open()

# OPEN AND READ MACHINE DESCRIPTION DATA
mach_descr = imas.DBEntry(MDSPLUS_BACKEND,database_md,shot_md,run_md,user_md)
mach_descr.open()
interferometer_md = mach_descr.get('interferometer')

# CREATE LOCAL OUTPUT DATAFILE
output = imas.DBEntry(MDSPLUS_BACKEND,database_out,shot_out,run_out,user_out)
output.create()

# TIME ARRAY
time_array = scenario.partial_get(ids_name='equilibrium',data_path='time')
ntime = len(time_array)

# START TIME LOOP
first_time_slice = 1
for itime in range(ntime):

    # TIME PASSING BY
    print('Time = %5.2f' % time_array[itime],'s, itime = ',itime,'/',ntime)

    # GET EQUILIBRIUM AND CORE_PROFILES FOR CURRENT TIME SLICE
    equilibrium_scen   = scenario.get_slice('equilibrium',  time_array[itime],CLOSEST_SAMPLE)
    core_profiles_scen = scenario.get_slice('core_profiles',time_array[itime],CLOSEST_SAMPLE)

    # RUN THE SYNTHETIC DIAGNOSTIC
    interferometer_out = dip_tip(equilibrium_scen,core_profiles_scen,interferometer_md,'parameters.xml')

    # SAVE OUTPUT TO LOCAL DATABASE
    if first_time_slice == 1:
        output.put(interferometer_out) # !!! FOR STATIC DATA TO BE SAVED
    else:
        output.put_slice(interferometer_out)

    first_time_slice = 0

scenario.close()
mach_desc.close()
output.close()

print('Done.')
```

Specify database entries for reading plasma scenario, machine description data, and storing output

Open scenario database, read machine description data, and create output database entry

Read equilibrium and core_profiles IDSs

Run synthetic diagnostic

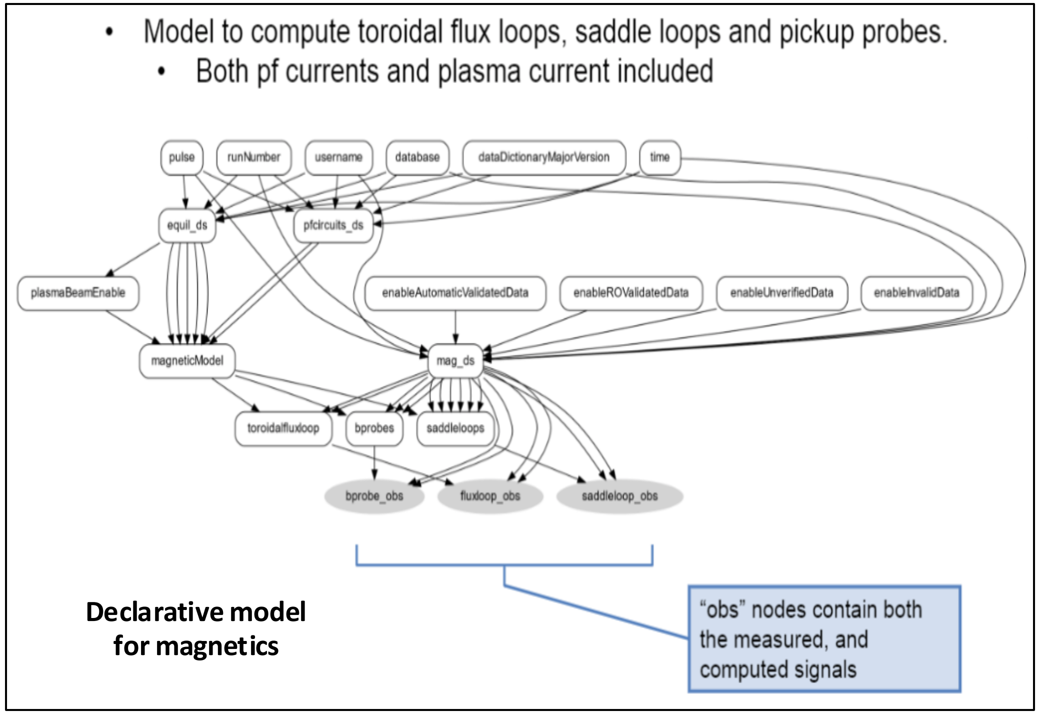
Save output

Loop over time slices

Synthetic diagnostics in Minerva

EURO SLING

- Initial focus on diagnostics models for First Plasma and PFPO operation
- Associated Machine Description data (being populated):
  - Magnetic coils, flux loops, Rogowski loops:
    - input = magnetics, pf_active, pf_passive, equilibrium
    - output = magnetics
  - VSRS, H-alpha:
    - spectrometer_visible
  - interferometry:
    - interferometer
  - X-ray spectrometer (edge/core/survey):
    - x_ray_crystal_spectrometer



- Early application:
  - Assessment of diagnostic coverage for early detection of L-H transition in PFPO-2
    → See talk by Anna Medvedeva on Friday

Thank you!

Europe’s first ITER Vacuum Vessel sector is complete!

EuroHPC
Joint Undertaking

REPUBLIC OF SLOVENIA
MINISTRY OF HIGHER EDUCATION, SCIENCE AND INNOVATION

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