IMAS Data Dictionary: an Introduction

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What is IMAS ?

- IMAS is the ITER Integrated Modelling and Analysis Suite
- Infrastructure :
  - Data Dictionary : a machine generic ontology for magnetic fusion :
    - What data exist ?
    - What are they called ?
    - How are they structured ?
  - Data Access : functions to read/write objects defined in the Data Dictionary (available in Fortran, C++, Python, Matlab, Java)
  - Workflow component generator : encapsulate physics codes (using IDSs as I/O) to turn them into components that can be coupled in a workflow
- Physics applications : components and workflows (e.g. ETS, HFPS, …)

The IMAS Data Dictionary : a fusion standard

- The IMAS backbone is a machine-generic ontology : the physics Data Dictionary
  - Capable of covering all experiment subsystems and plasma physics, and is extensible
  - It represents simulation and experimental data with the same data structures, enabling direct comparisons
  - The Interface Data Structures (IDSs) are specific entry points of the Data Dictionary. They typically describe a tokamak subsystem (diagnostic, heating system, …) or an abstract physical concept (equilibrium, set of plasma profiles, wave propagation, MHD, …)
  - They define standard interfaces between physics components in an IMAS workflow
- The IMAS Data Dictionary is being promoted as the standard to enable Interoperability in the FAIR and open science requirements for FP9 (Fair4Fusion project, EUROfusion Data Management Plan)
- The IMAS Data Dictionary and Access Layer are now available Open Source

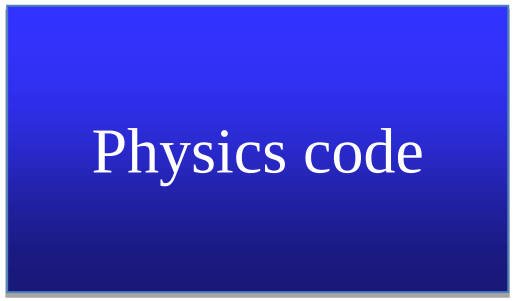
What TSVVs and DTE can do with the IMAS infrastructure ?

- **Share/store/publish data using a fusion-standard ontology**
  - Store simulations results and compare to an experiment
  - Exchange simulation results with other codes (benchmarking, reuse of input datasets)
  - Create a catalogue of simulations that can be searched/browsed (various catalogue prototypes are under development : simDB, DMP, …)
  - Make data FAIR and Open

- **Assemble a workflow of physics components** (Integrated Modelling, Simulation post-processing, Plasma Reconstruction Chains, …)
  - E.g. process synthetic diagnostic output from a simulation and compare to an experiment

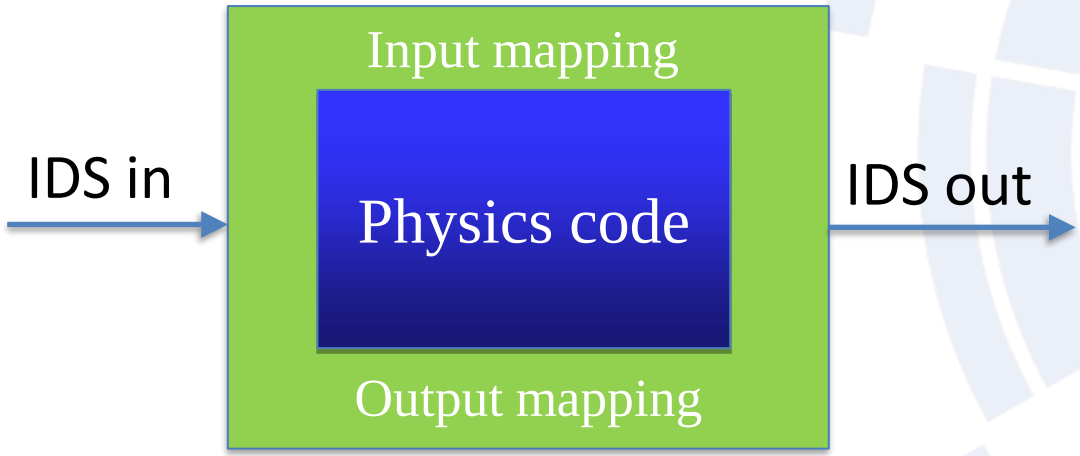
IMAS integration steps

- Step 0 : the physics code



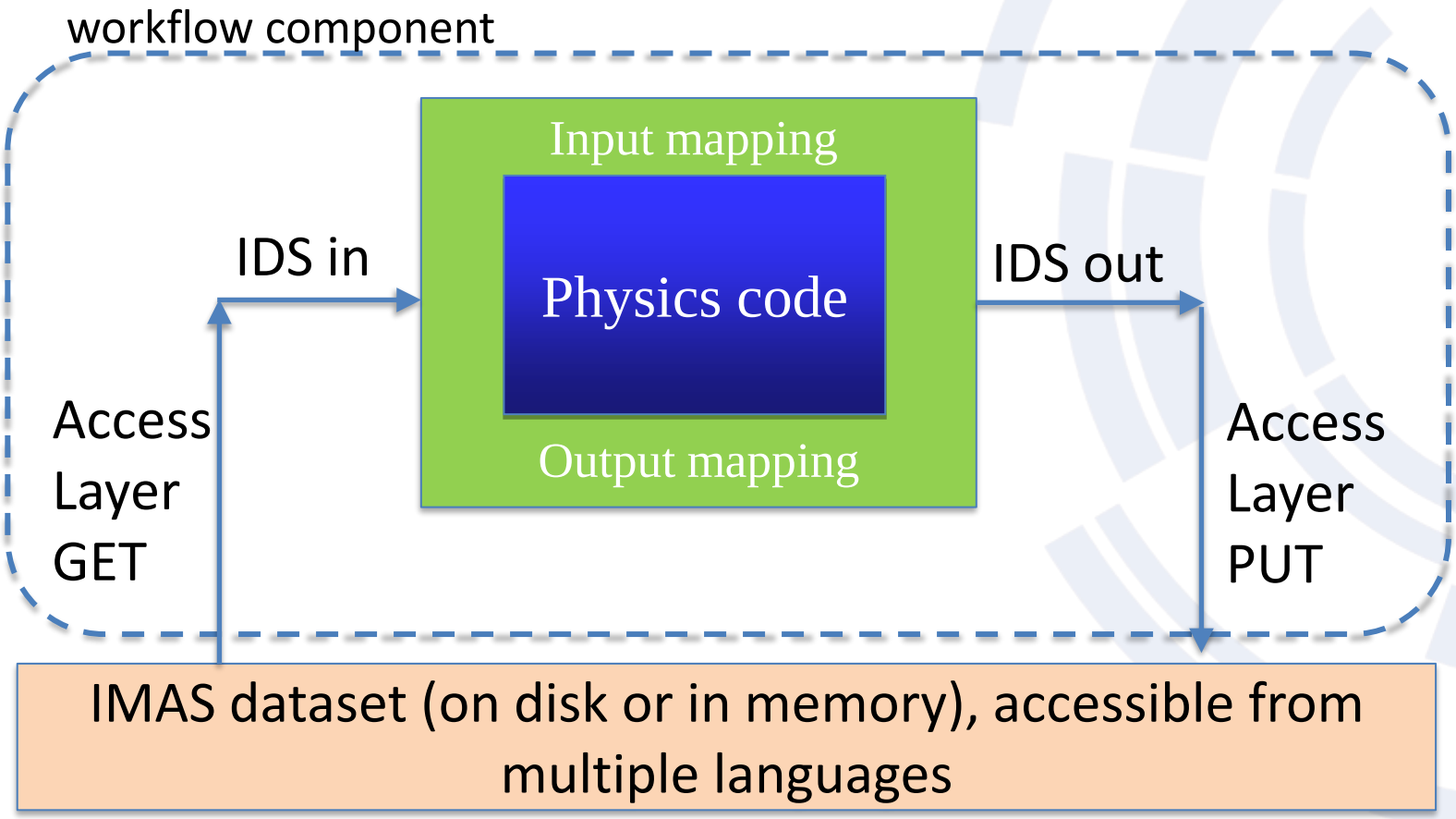
IMAS integration steps

- Step 1 : the TSVV physics code with I/O mapped to IMAS Data Dictionary



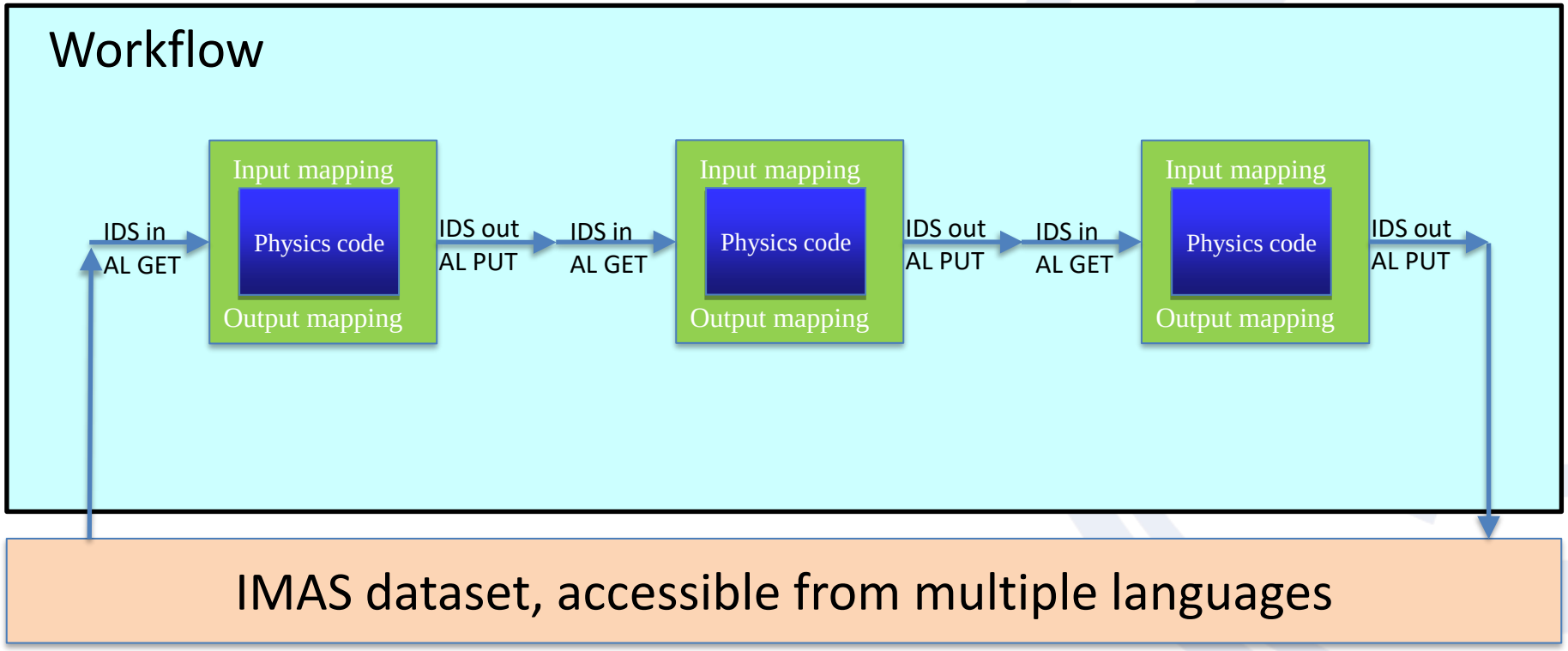
IMAS integration steps

- Step 2 : the physics code with I/O mapped to IMAS Data Dictionary uses the Access Layer to read/write data
- NB : this step, encapsulated, results in a potential workflow component



IMAS integration steps

- Step 3: multiple physics code with I/O mapped to IMAS Data Dictionary use the Access Layer to communicate together in a workflow



What means « adapting a code to IMAS » ?

- Basic level (minimal requirement for EUROfusion standard software)
  - Agree on a minimal set of input/output data to be mapped to IMAS
  - Create mapping script that will do the mapping and read/write data to an IMAS database
- Full IMAS interface
  - Map full I/O to IMAS, including code-specific parameters, and optionally restart files as well
- IMAS component
  - Full IMAS interface + generate component directly usable in workflows (Python, Muscle 3, …)

You may have needs that are not covered yet by the IMAS Data Dictionary

- You may contribute to the Data Dictionary !
- The IMAS Data Dictionary is extensible
- It has precise lifecycle procedure to be able to evolve and be jointly developed by multiple teams
- It has precise design rules to ensure global homogeneity
- Question/feature request ? : go to https://github.com/iterorganization/imas-data-dictionary and create an “issue” or a “discussion” → the repository is open !

Now we pause for questions before …

Going deeper inside the IMAS DD structure

Deeper insight : Interface Data Structure

- The Data Dictionary has a tree structure, for the sake of clarity
- At the top level, a collection of modular structures (IDSs) representing
  - Abstract physical quantities (e.g. distribution functions)
  - Tokamak subsystems (e.g. PF systems)
- By default, data access is made at the level of these structures (Write and Read)
  - NB : Partial Get is now available to read only a subset of an IDS structure
- These modular structures have the appropriate granularity for exchange in an IM workflow → they also represent standardised interfaces for communication between codes, named Interface Data Structure (IDS)
  - Each has an “ids_properties” substructure (metadata + comments + timebase usage)
  - Each has a “code” substructure (trace the code-specific parameters and the name/version of the code that has generated this IDS)

Data Dictionary documentation

- Openly available here : https://imas-data-dictionary.readthedocs.io/en/latest/reference_ids.html
- The IDS reference first shows the list of all IDSs. For each of them, a detailed documentation:
  - Full path name: name of all variables of the IDSs, with their path in the structure. **Replace "/" by the structure operator in a programming language, e.g. "%" in Fortran (core_profiles%global_quantities%ip), "." in C++, Matlab, Java, Python (core_profiles.global_quantities.ip)**
  - Definition
  - Units
  - In {}, whether it is STATIC (constant over a range of pulses, e.g. machine configuration), CONSTANT (constant over the pulse or the simulation), or DYNAMIC (time-dependent within the pulse or the simulation)
  - Data_Type in Blue: indicates whether it is a string, an integer or a real, and its dimension (0D, 1D, 2D, …)
  - Coordinates: for each dimension, the full path name to the related coordinate. If the dimension simply refers to a quantity not present in the Data Model, it is indicated as "1…N"
  - DD lifecycle information
- Also on this site: search DD tools, IDS migration guide, GGD guide, DD developer documentation

Timebases in IDSs

- “time” is a reserved node name for any timebase in the DD. Such nodes are recognized and used by the Access Layer when getting or putting time slices (GET_SLICE / PUT_SLICE functions).
- An IDS may contain quantities with different timebases in order to have the ability to describe experimental data as it is acquired in the experiment.
- However, an IDS can also be filled in a synchronous way (i.e. all dynamic quantities are stored on a unique timebase, located at the root of the IDS)
- There are therefore two possible usages of the IDS, with two possible locations for the “time” coordinate related to a given node. **Homogeneous_time is set by the data provider**.

Value of ids_properties/homogeneous_time	Location of the time coordinate for dynamic nodes
0	Dynamic nodes may be asynchronous, their timebase is located as indicated in the “Coordinates” column of the documentation.
1	All dynamic nodes are synchronous, their common timebase is the “time” node located at the IDS root (e.g. equilibrium/time).
2	Means that no dynamic node is filled in the IDS (dynamic nodes will skipped by the Access Layer)

You don’t need to fill everything when writing an IDS

- An IDS can contain a fairly large number of physical quantities and covers a wide range of use cases. Therefore there will be many cases in which the IDSs are only partially filled.
- The only requirement regarding empty fields are:
  - The ids_properties/homogeneous_time field must be filled (unless the IDS is static)
    - If homogeneous_time = 1, the root time must be filled
  - When a quantity is filled, the coordinates of this quantity must be filled as well
- Not meeting these requirements will cause PUT methods to return an error.

Arrays of structure

- Arrays of structures are frequently used in IDSs, to describe a list of elements that may have nodes of different sizes, in order to avoid creating large sparse arrays
- The two typical cases are :
- Case 1: lists of objects that may contain asynchronous nodes, e.g. PF coils may be acquired with different timebases :
  - pf_active%coil(i)%current%data(itime)
  - pf_active%coil(i)%current%time(itime)
  - These Case 1 AoS are used essentially in IDSs representing tokamak subsystems
- Case 2: list of time slices. The structure contains only dynamic and synchronous nodes, e.g. equilibrium/time_slice(:). This time slice representation allows the size of the children to vary as a function of time (e.g. variable grid size). These Case 2 AoS are used essentially in IDSs representing abstract physical quantities

Lifecycle information

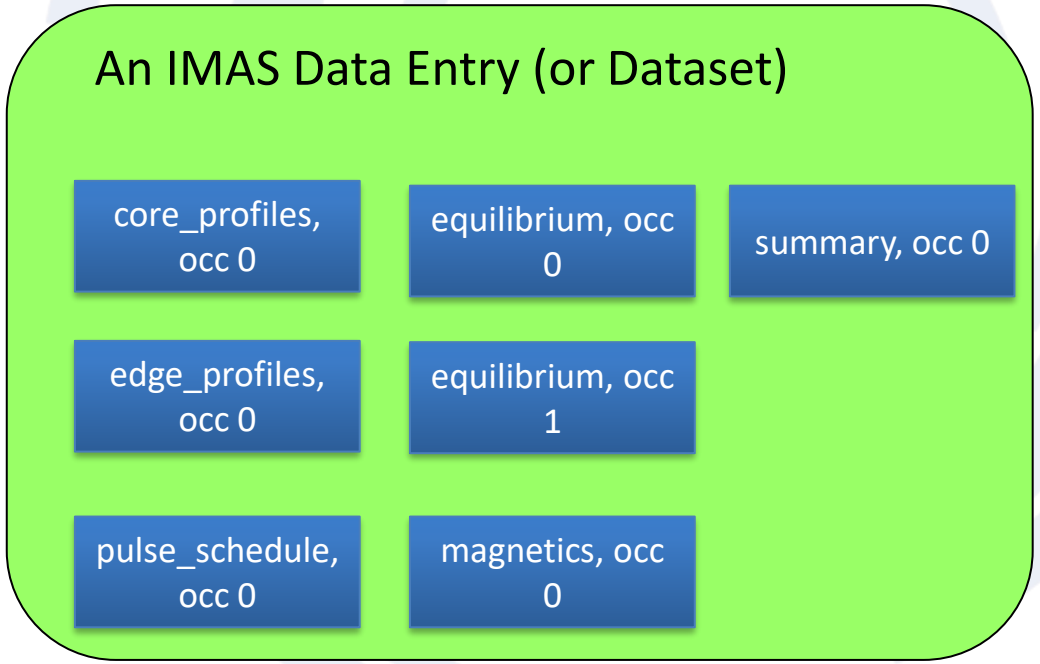
- The DD is a living object that evolves and expands with the needs. Therefore the lifecycle status of each node is documented
  - Some parts of the DD are recent and may evolve rapidly “lifecycle_status = alpha”
  - Some other parts are used for a longer time and are more stable “lifecycle_status = active”. If they need to be changed, they will become “obsolescent” but will not suddenly disappear (until a Major Release)
  - Some other parts are deprecated and shouldn’t be used “lifecycle_status = obsolescent”
- The lifecycle status of IDS nodes is described in the documentation. It applies to all descendants of a node, unless a descendant carries a different lifecycle status
- Two major versions are currently used
  - DD v3 (latest 3.42.2): mostly used outside of IO – frozen since 2024 (only technical patches allowed)
  - DD v4 (latest 4.1.1): used at IO – some non-backward compatibles changes w.r.t. v3 – allowed to evolve

Now we move to …

IMAS Data entries

IMAS Data Entries for storing simulation input/output

- A Data Entry is a collection of IDSs, gathered as a logical dataset (e.g. all IDSs corresponding to a given simulation output)
- A specific IDS, “summary” is the placeholder for description of the content of the dataset
- Multiple occurrences of a given IDS can co-exist, e.g. multiple equilibria calculated by different codes / assumptions
- Historically a Data Entry is defined (similarly as a pulse dataset in an experimental database) by:
  - IMAS “major version” (=“3” or “4”)
  - User name
  - Machine name
  - Pulse number
  - Run number (multiple simulations related to the same pulse)
- With recent versions of the Access Layer, a data entry is defined via a URI in a more generic way:
  - imas:[//host/]backend?query[#fragment]
  - imas:mdsplus?pulse=123;run=2;user=public;database=ITER;version=3
  - imas:hdf5?path=/home/username/runfolder
  - imas:ascii?path=./debug
- Choose a File Backend to write to disk (MDS+, ASCII, HDF5)
  - Create or open a Data Entry
  - Then GET or PUT individual IDSs from/in it

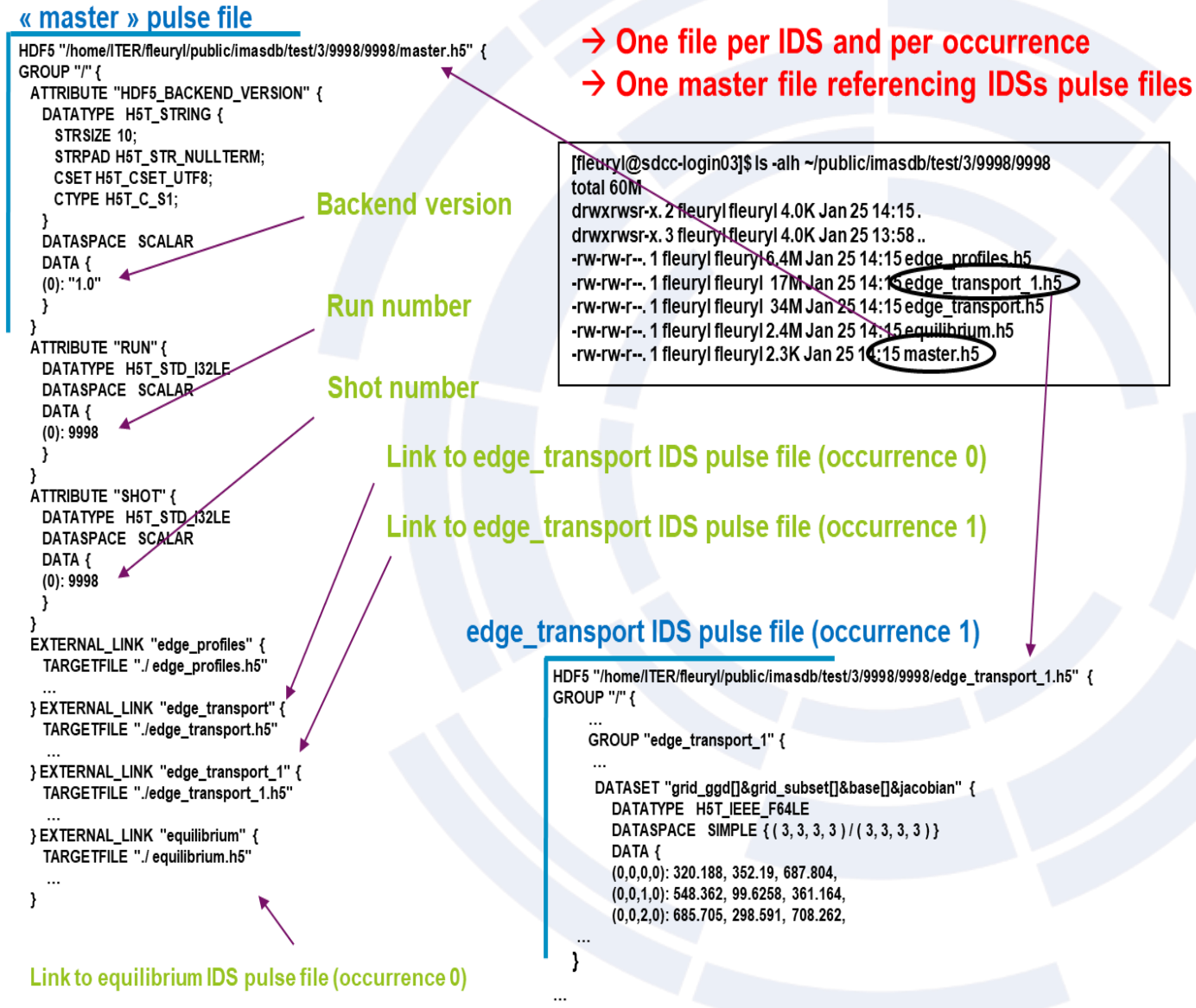


Which IMAS Backend to use ?

- Three Backends are available to write IMAS data to files
  - HDF5 Backend is the most recent and most optimized Backend for IMAS → we recommend using this one to produce new datasets
  - MDS+ Backend it the historical one, many datasets are available with this backend. Drawback : creates huge data files even for small amounts of data
  - ASCII Backend is not recommended for large data size, but may be interesting for rapid testing purposes. Reduced functionalities (no time slice operation)
- There are also other Backends
  - Memory Backend allows faster exchange of IDSs in memory (e.g. between components written in different languages)
  - UDA Backend allows reading (not writing, so far) data remotely, and includes an optional data mapping step (e.g. for reading experimental data not natively in IMAS format)
- There is also a NetCDF export function in IMAS-Python but it changes the data format (tensorization), to be used to export data to non-IMAS users. No time slice operation

IMAS file structure when using the HDF5 Backend

- If using the “legacy” Data Entry definitions: all pulse files are located in the user’s account under the folder: ~/public/imasdb/DatabaseName/IMASMajorVersion/SHOT/RUN
- Otherwise they are located under the folder you specified
- Modular organization:
- One file per IDS and occurrence
- One master file with the references



Conclusion : you are ready to start playing with IMAS

- The IMAS infrastructure features a standard, machine-generic Data Dictionary for experiment and simulation data, together with an Access Layer in multiple programming languages
- ITER Organization succeeded to make it a true fusion standard among ITER members
- IMAS facilitates:
  - Building FAIR fusion databases
  - Sharing data accross experiments and simulation tools
  - Interfacing codes

- Data Dictionary documentation: https://imas-data-dictionary.readthedocs.io/en/latest/reference_ids.html
- Question/feature request ? : go to https://github.com/iterorganization/imas-data-dictionary and create an “issue” or a “discussion”
- All Open Source
- See next courses for an Introduction to Access Layer in Python and Matlab
- Our ACH can support you during your usage of IMAS

BACKUP SLIDES

- BACKUP SLIDES

Minimal workflow for reading from / writing to IMAS
In green : what the TSVVs have to do

- The IMAS infrastructure has an API (Access Layer, AL) to read (GET) and write (PUT) IDS structures from a variable in your favorite language (Fortran, C++, Matlab, Python, Java) to a file (MDS+, ASCII, HDF5).
- OPEN the data entry of interest (for your input)
- GET the IDSs of interest for the input to your code
- Map the IMAS input to your code's data model
- Run your code
- Map your code output to IMAS
- OPEN/CREATE your output data entry
- PUT the output IDSs to the output data entry
- CLOSE data entries
- You are done !