

Overview of WP Code Development activities in 2020-2021

Pär Strand, and the WPCD team





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CHALMERS

Outline



General remarks on WP CD activities

A select set of highlights and developments from

- IMASification activities
- Exploitation activities
- Development

Not a complete review – not possible due to time constraints





WP Code Development officially ended 2020 - some lingering activities in 2021 due to COVID delays:

- Make data-structure (IMAS / IDS) and workflows developed by WPCD available to USERS in EUROfusion for routine analysis and modelling across EUROfusion programs / laboratories
- Demonstrate the added value of using the Integrated Modeling (WPCD) tools by supporting their use in JET /MST for delivering new scientific results

WPCD workflows as tools for USERS and not exclusively for developers

Some activities within new eTasc structure (TSVVs and ACHs) with reduced level of users support maintained.



WPCD in collaboration with CPT built applications on the Integrated Tokamak Modelling Taskforce toolsets (CPOs, UAL, FC2K,...) and rebased these towards IMAS (IDS, AL, FC2K,...)

AIMS

- **Bring data to users:** Implementing and supporting access methodologies for EUROfusion devices (Machine descriptions, data mappings and access)
- Bring tools to users: Deployment of workflows and data analysis tools
- Bring skills to users: User support, training and documentation and
- Bring feedback from users: New requirements, updates and bugfixes



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| ITM-TF | \rightarrow | WP CD | \rightarrow | ITER/IMAS |
|------------|---------------|--------------|---------------|------------|
| Innovation | | Evolution | | Deployment |
| Invention | | Diffusion | | Acceptance |
| | | (production) | | Production |



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ITM-TF Innovation Invention WP CD

 \rightarrow

Evolution Diffusion (production) ITER/IMAS

Deployment Acceptance <u>Production</u> Are we (ITER) suffiently well resourced and structured for this? CD-IO meeting



- Bring data to users: Implementing and supporting access methodologies for EUROfusion devices (Machine descriptions, data mappings and access)
 - UDA (In principle available but yet to be fully established as a general tool)
 - Bespoke toolset used to map data from experiments.
 - Exp2itm, Trview (for AUG data), readAUG, IMASgo! (Omfit plugin), TCV2IDS,...



ITER could be an incubator for the IMAS/UDA paradigm. In general, little interest from experiments otherwise to engage.





CD-IO meeting

| IDS Name | JET | TCV | AUG | MAST | WEST |
|--------------------|-----|-----|-----|------|------|
| iron_core | | | | | |
| magnetics | | | | | |
| mse | | | | | |
| pf_active | | | | | |
| tf | | | | | |
| thomson_scattering | | | | | |
| wall | | | | | |
| core_profiles | | | | | |
| equilibrium | | | | | |
| nbi | | | | | |
| ic_antennnas | | | | | |
| ec_antennnas | | | | | |
| core_sources | | | | | |

| Colour | Meaning |
|--------|--|
| | Data not relevant for this machine |
| | Data is missing |
| | Data mapping in development |
| | Data available |
| | Data validated as input of EWE-2 and EWE-3 workflows |

- Initial experimental input datasets provided for "all" EUROfusion machines
- Iterative process with workflow owners to test / extend the datasets as required
- Alternates to UDA to process native data and map them in IMAS/IDS have been developed to target specific workflows:
 - TRVIEW
 - IMASgo
 - TCV2IDS
 - ReadAUG-



| IDS Name | JET | TCV | AUG | MAST | WEST |
|--------------------|-----|-----|-----|------|------|
| iron_core | | | | | |
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| pf_active | | | | | |
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| core_profiles | | | | | |
| equilibrium | | | | | |
| nbi | | | | | |
| ic_antennnas | | | | | |
| ec_antennnas | | | | | |
| core_sources | | | | | |

TRVIEW (AUG)updates and features:

- New Gaussian spline method
- Toroidal velocity profiles have been made available (there was a bug before)
- Zeff time traces made reliably written
- Map full equilibrium to IMAS, including COCOS recognition and conversion
- Main species recognition
- Added RABBIT input
- Added angular frequency as option instead of vtor (user's choice)
- Usable also on AUG reversed Ip/Bt shots

| Colour | Meaning |
|--------|--|
| | Data not relevant for this machine |
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TRVIEW is also used for ASTRA and TRANSP



| IDS Name | JET | тси | AUG | MAST | WEST |
|---|-----|-----|-----|------|------|
| iron_core | | | | | |
| magnetics | | | | | |
| mse | | | | | |
| pf_active | | | | | |
| tf | | | | | |
| thomson_scattering | | | | | |
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| core_profiles | | | | | |
| equilibrium | | | | | |
| nbi | | | | | |
| ic_antennnas | | | | | |
| ec_antennnas | | | | | |
| core_sources | | | | | |
| Colour Meaning Data not relevant for this machine Data is missing | | | | / | |

WEST data is native IMAS and available through UDA

te velideted as input of EWE-2 and EWE-3 workflow

IMASGO updates and features:

- OMFIT plugin for ETS level input data
- Used for MAST, JET, DIII-D and K-Star data preparation

IMAS/UDA (magnetics data for EWE-2).

- MSE and Thomson-Scattering data available for both JET and MAST.
- Interferometry made available MAST UDA
- JET plugin development (allowing private PPF instances not only public).
 - This was useful for e.g. MSE data at JET which is processed manually by individuals outside of the standard Plasma Reconstruction Chain.
- Data for existing EFIT Equilibria is available for both JET and MAST.
- NBI mappings are in progress for MAST but are not yet available.



| IDS Name | JET | TCV | AUG | MAST | WEST |
|--------------------|-----|-----|-----|------|------|
| iron_core | | | | | |
| magnetics | | | | | |
| mse | | | | | |
| pf_active | | | | | |
| tf | | | | | |
| thomson_scattering | | | | | |
| wall | | | | | |
| core_profiles | | | | | |
| equilibrium | | | | | |
| nbi | | | | | |
| ic_antennnas | | | | | |
| ec_antennnas | | | | | |
| core_sources | | | | | |

Data not relevant for this machine

Data validated as input of EWE-2 and EWE-3 workflows

Data is missing Data mapping in development

Data available

TCV2IDS

Updated data mappings required by the equilibrium reconstruction and stability workflows:

- magnetics
- pf_active
- tf,
- wall
- equilibrium
- core_profiles
- thomson_scattering (new IDS)

Data required for ETS simulations has also been added:

- ec_launchers
- nbi,
- summary ids.

These 10 IDSs are the present default set for tcv2ids2 database, working on both the gateway and ITER-IO.



- Bring tools to users: Deployment of workflows and data analysis tools
 - ETS (5 \rightarrow 6), EQRECONSTRUCT, EQSTABIL, (EDGETURB) [EWE-2 and EWE-3]
 - Full ecology for interpretative/predictive analysis
 - Multiple interfaces: autoGui, (front end Gui), Canvas (Kepler layer), ETSviz+other scripts,



struct



IMAS Version: 6.2.0 RECONSTRUCTION Select the time of interest ("time_begin", "time_end" and "time_dt" variables) Reconstruct equilibrium using EQUAL, NICE (EFIT++ or CLISTE in the forge) codes. DDF Director Cut-off the reconstructed equilibrium for fixed boundary high resolution calculation Calculate high res. equilibrium with codes : HELENA, CHEASE and CAXE SAVE SLICE ADVANCE Check TIME

CHECK DATA

START

Equilibrium Reconstruction Workflow

Workflow uses data from arbitrary tokamak devices and accommodates "arbitrary" plasma equilibrium reconstruction codes adhering to IMAS.

- Default codes EQUAL and NICE
- Operational modes depends on available data:
 - In the more basic mode, only data from magnetic sensors/coils is used, possibly complemented by Faraday rotation or Motional Stark Effect data.
 - At a second (optional) stage, the thermal plasma pressure can be used for a refined reconstruction (to capture pedestal relevant features)

The workflow was used successfully to address typical uses cases from JET, AUG and TCV devices.

STOP THE RUN

It was also attempted on MAST, WEST and KSTAR devices but with little success except very preliminary for MAST. (Cocos adherence apparently hard to maintain).



A negative triangularity case with separatrix, TCV



Good agreement is found between the several codes (LIUQE – the in-house tool at TCV, EQUAL and NICE). Comparison of flux contours, magnetic probe and flux loop reconstruction errors and obtained |q| profiles for the codes LIUQE, EQUAL and NICE using data from TCV discharge 67455 at t = 0.7s. Black dashed lines indicate the absolute error for the different signals



AUG validation/bechmarking with CLISTE on shot 33173



Comparison of flux contours, magnetic probe and flux loop reconstruction errors and obtained |q| profiles for the codes CLISTE, EQUAL and NIICE using data from AUG discharge 33173 at t = 3.0s. Note that the reconstruction errors for CLISTE are missing since this data hasn't been mapped to IDS format. Improvements are possible since no fine-tuning was done for the sensitive code parameters e.g. knot positions and weigths for the regularisation.







Comparison of flux contours, magnetic probe and flux loop reconstruction errors and obtained pressure profiles for the codes EFTP, EQUAL and NICE using data from JET discharge 84600 at t =51.0s. Similarly to CLISTE in figure 3, reconstruction errors are missing for EFTP (branding at JET for EFIT++ constrained with plasma pressure). The closer agreement of EQUAL and EFIT++ may be justified by the closer solver kernel used, both derivations of the EFIT algorithm, whereas NICE uses a rather different approach. UDA mapping updates needed to match magnetics between EFTP and IMAS CD-IO meeting



The linear MHD stability is a single time slice

analysis workflow so that I can be easily

integrated into larger scope workflows,(ETS or in

EQRECONSTRUCT).

Equilibrium codes used

HELENA, CHEASE and CAXE,

updated to the latest DD versions. It couples

stability codes

- Kinx (with Caxe)
- ILSA, MARS and MARS-F (HELENA and

CHEASE)

The workflow was used routinely to analyse the MHD stability of plasma from several devices including JT-60SA in the framework of a task in WPSA

IMAS

Version: 6.2.0

High resolution equilibrium

- Starting from free boundary equilibrium reconstruction or fixed boundary calculated equilibrium.
- Option to define new plasma boundary inside the separatrix.
 Calculate high res. equilibrium with codes : HELENA, CHEASE and CAXE.
- Laiculate high res. equilibrium with codes : HELENA, CHEASE and

Linear MHD stability workflow

MHD stability

- Calculate linear MHD stability for a given toroidal mode number(s) with MHD codes : ILSA, MARS, or KINX
- Interchangeability between HELENA and CHEASE when using ILSA, MARS codes.
- Plotting of equilibrium flux map, plasma profiles and MHD eigenfunctions.





Application to MAST on shot 27205



High resolution equilibrium from MAST (#27205 at t=0.4s) and linear eigenfunction for "radial" velocity component for a n=1 internal kink mode. Input data from IMASgo stored in g2mroma/MAST/27205/1 and HELENA and ILSA codes were used



Application to JT-60SA, Scenario 4 with data mapped from eqdsk file, (hybrid scenario with internal transport barrier in ion energy channel). The scenario is characterised by internal infernal like modes where the ITB is located (as found in analysis).



Normalised growth rate scaling with toroidal mode number (left) and radial velocity component of the most unstable mode (right) are shown for the CDBM equilibrium with fast ion pressure included.



- CLISTE as a Kepler actor: A Python actor plays the interface role between the IMAS database and CLISTE. The main advantage being that any change in either CPOs or IDSs (IMAS) can be solved inside this Python actor. Moreover, the original CLISTE code can be used without having to deal with different CLISTE versions.
- Intermediate step towards having the whole CLISTE suite interfaced to IDSs

Imasification of CLISTE deemed to resource demanding in view of the compliance to both IDSs and the ASDEX Upgrade environment system and dedicated shotfile system – CLISTE is the de facto intrashot code used in the Research programme of AUG.



The KEPLER test workflow for the CLISTE code driven by a UALPython actor. In the particular case, a TCV test case is considered (previously tested in the standalone code)

CLISTEPATH: /marconi/eufus_gw/home/g2egiova/Garching/python_spwaner



 The integration and testing of EFIT++ in IMAS was severely hampered by extraordinarily long linking times during the build process of the code and actor. Although this was prioritised and support from the CPT was secured, the underlying cause remained unclear though potential culprits might involve either the UAL C++ HLI and/or the massive use of templates by EFIT++ (or both).



- Fundamental atomic calculations have been performed for Ne like Mo.
- Extensive calculations have been done on electron backscattering from Be, Be4+ and hydrogen atom and between hydrogen atoms has been performed.
- Significant work has been done on collecting and using atomic cross-section data. JET results seem to
 indicate that the previously developed T-T nuclear cross section provides a significantly better description
 than previous cross-sections
- It is not clear what, if any, future exists for AMNS work within EUROfusion with the termination of WPCD.
- It is also not clear what the plans are for the future maintenance of the AMNS library and the curation of future AMNS data.
- More work in the area of cross-sections and nuclear data could usefully be performed in the future, as well as the completion of the beam-stopping work.
- The incorporation and extension of surface data from the CPO version into the IDS version still remains to be done

AMNS data and interfaces in IMAS



Updating of the W data for the CPO version



While the W data for the IDS version had been updated, development work had stopped for the CPO version. In comparisons of the ETS-5 with other calculations this issue was identified and the W data was then updated. The left figure used older W data and the right a newer version. The calculated radiation increased by ~55%. CMP ETS implementation and testing

Calculation of new T-T crosssection data tested at JET:

In previous work done as part of WPCD and JET activities, the existing nuclear data for T-T reactions was examined. Since the available data disagreed, a new parameterisation was prepared based on ENDF data.

BEAST T plasma results

 98551 - Checking dependency of fusion rate on T density and XS



New results from JET suggest that this data is in better agreement with the experimental measurements than the previous data used in TRANSP.



Aimis to provide plug-ins for visualization tools developed by WPISA:

- Enhanced ParaView plugin for Edge IDSs (Edge Profiles, Edge Sources, Edge Transport) and MHD IDS (under SOLPS-ITER GUI Git)
- IMASviz plugins template and documentation for dashboard inclusion and documentation with template of a simple plugin.
- Plugins for SOLPS, ETS (under IMASViz Git).
- ParaView plugins (GGD based) in separate Git
- ETS plugin for IMASViz (not finalized)
- Support for other IDSs (e.g. Eqstabil workflow)
- AppImage support (Raysect, Cherab) under SMITER GUI

Visualization tools in IMAS





ReadUALGGD ParaView plugin

The ReadUALEdge ParaView plugin was initially intended for passing the data from Edge Profiles, Edge Transport and Edge Sources Interface Data Structures (IDSs) to ParaView

SOLPS-ITER, EDGE2D

Overview of IMASViz interface and its available features

Implementing the Multiple Document Interface (MDI) in IMASViz, allowing better arrangement of the panels and windows under a single main window



CD-IO meeting



- An open-source python library ToFU, to be used as a numerical toolbox for synthetic diagnostics on Tokamaks, called tofu, was developed (and continues to be developed), providing a production-ready tool to users on EUROfusion devices and ITER.
- In use at ITER to compute synthetic signal from the prospective ITER bolometry. WEST for other diagnostics thanks to its generic tools and algorithms.
- It is also unit-tested, natively compatible with IMAS and numerically optimized (parallelized), and provides online sources and documentation and bash commands for simple uses for users who are not familiar with python.
- https://tofuproject.github.io/tofu/releases.html.



Several versions of tofu were released during the year.

- New default tokamak geometries (ITER, AUG, WEST, TCV...)
- Faster algorithms (optimized / parallelized using cython)
 Additional features (handling of basic reflexion mechanisms, interactive plotting)
- Debugging and maintenance
- Features added to satisfy user-feedback (better interactivity of figures, more explicit error messages...)
- IMAS compatibility
- Unit tests
- Documentation updating
- mplementation of coding good practices (coding style conventions, docstrings, comments...)
- Deployment of the library (to very popular online python repositories like Pipy and Conda) to make installation an easy as possible, using pip install tofu ro conda install –c conda-forge tof



European Transport Simulator



Work on ETS related physics modules and ETS workflow and its exploitation was a significant part of the of the WPCD activities and work relating to WIMAS-2, WIMAS-5 and EWE-3 is reported here in addition to the related work by The ETS TRO.



European Transport Simulator



ETS currently exists in two flavours:

- ETS v5 (CPO based version, being phased out)
- ETS v6 (IMAS based version, being phased in)

ETS v6 is more than a simple remapping of ETS v5 to a new data format – extended and adapted based on user requriements and lessons learned.



European Transport Simulator





Transition to ETS v6 slowed down by the Covid-19 situation

- Small part of WPCD continued until end June 2021.
- WPISA (CPT) workflow support continued until end June 2021.

Qualification of new releases somewhat affected

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ETS v5 will be kept for verification purposes as long as needed Users will be supported to move to ETS v6



European Transport Simulator



Horizon Europe

WPCD is dispersed in FP9 but support continues from the advanced computing hub Structure for ETS, EQSTAB and EQreconstruct. The IM modelling hub (IPPLM/PSNC) provides

- Workflow support and maintenance
- IMASification of new physics models

The ETS community will be supported by

- Direct support from the IM ACH hub ETS support staff
- An improved online support structure/presence
- Weekly users/developers meetings (starting after summer vacations in earnest)



The move to IMAS required not only shifting all physics modules and supporting actors from CPOs to IDS but also required changes to the workflow (code) logics.

In addition, improvements on user interfaces to support the end user experience. ETS is highly modular and the user interfaces provide access to almost all configurable aspects of the workflow and the physics modules used.



Two interfaces available: Kepler Canvas interface (above) which provides an excellent overview of software relations including configurations (and has a Powerful shortcut system for expert users).



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| | OCC 2: Profiles update | d during iteratio | TURBULENCI | E TRANSPORT: | Please choose (Off - no turbule | turbulence trans ence transport wi | sport model to be rill be called) | used | | | | | | |
|--------------------------------------|--|-------------------|-----------------------|--|---|---------------------------------------|--------------------------------------|---------------------|-------------------------------|------|----------------|----------------|----------------|-------------------------------|
| | EQUILIBRIUM | TRANSPORT | cal | ling frequency: time intervals: | TGLF Please choose t every iteratio | frequency for ca | lling turbulence ti | ransport | 1-D TRANSPORT EQUATIONS | EDGE | CON | RGENCE | new converting | erged solution core PLASMA |
| | | - | NEOCLASSIC | AL TRANSPORT: | Please choose (Off - no neocla | neoclassical trar | nsport model to b will be called) | e used | | | , | COMMERCISIO | OCC 2 | |
| | | | cal | Model: ling frequency: time intervals: | NCLASS Please choose f every iteratio | , frequency for cal n | lling neoclassical | transport | | | rt cowtroop en | T COWERGED RES | | |
| | 04-20001 | | DATA BASE 1 Data E | FRANSPORT ==: Base Transport: | Please choose | if transport coeff | ficients saved to i | nput shot/run mu | | | P ITOM TA | AT THE STOP | | |
| | new -> OCC 2 | | cal | lling frequency: time intervals: | Please choose every iteratio | frequency for ca | lling data base tr | ansport | | ne | w->0CC1 | 0001 | | |
| solution at previous time step | | | ADDITIONAL Additio | TRANSPORT =: onal Transport: | Please choose | if additional cons | stant transport co | pefficients must bi | | | | | | |
| | OCC1/2 ADT.COMERCED.REP. ITEMATING ADT.COM/GROED RESET TINE ST | s IP | cal | ling frequency: time intervals: | Please choose every iteratio 0.0 | frequency for ca | lling additional tra | ansport | | | | J | | |
| OCC 2 at later calls | | | Commit | Add | Remove | Defaults | Preferences | Help | | | | | | |

Two interfaces available: Kepler Canvas interface (above) which provides an excellent overview of software relations including configurations (and has a Powerful shortcut system for expert users).

solu at p time PLAS



The move to IMAS required not only shifting all physics modules and supporting actors from CPOs to IDS but also required changes to the workflow (code) logics.

In addition, improvements on user interfaces to support the end user experience. ETS is highly modular and the user interfaces provide access to almost all configurable aspects of the workflow and the physics modules used.

| OCC 2: Profiles updated during iteratio | TURBULENCE TRANSPORT: | Please choose turbulence transport model to be used (off on publicer transport will be called) | default tglf default | | |
|---|--|--|---|-----------------------|---|
| OCC 1: Profiles from the last converged | Model: | TGLF | - | | |
| | calling frequency: | Please choose frequency for calling turbulence transport every iteration | flags tglf_use_bper | ○ Yes ⑧ No | new converged solution for the core PLASMA |
| | time intervals: | 0.0 | tglf_use_bpar | 🔾 Yes 🖲 No | PLASMA_OUT |
| | NEOCLASSICAL TRANSPORT: | Please choose neoclassical transport model to be used | tglf_adiabatic_elec | 🔾 Yes 🖲 No | OCC 2 |
| | Model: | NCLASS | tglf_fastions | 🔾 Yes 🖲 No | |
| | calling frequency: | Please choose frequency for calling neoclassical transport every iteration | tglf_dump_flag | 🔾 Yes 🖲 No | |
| | time intervals: | 0.0 | tglf_calculate_angf | 🖲 Yes 🔾 No | |
| old -> OCC 1 new -> OCC 2 | DATA BASE TRANSPORT ==: Data Base Transport: calling frequency: time intervals: | Please choose if transport coefficients saved to input shot/run mu Off Please choose frequency for calling data base transport every iteration 0.0 | tglf_alpha_p tglf_alpha_e tglf_alpha_mach tglf_alpha_zf tglf_alpha_zf | 1 0 1 0 0 | |
| ion evious | ADDITIONAL TRANSPORT =: Additional Transport: | Please choose if additional constant transport coefficients must b | tglf_xnu_factor tglf_sat_rule | 1 0 | |
| MA_IN PLAMA OUT | calling frequency: time intervals: | Please choose frequency for calling additional transport every iteration 0.0 | tglf_full_wexb tglf_nbasis_max | 1 | |
| OCC 1 at his call OCC 2 at later calls | Commit Add | Remove Defaults Preferences Help | tglf_nions | 0 | |

Two interfaces available: Kepler Canvas interface (above) which provides an excellent overview of software relations including configurations (and has a Powerful shortcut system for expert users). Alternative: a flattened GUI! \rightarrow



The autoGui is automagically built form the loaded workflow and provides a flatter view of ETS and its settings and in addition has added features of launching and monitoring jobs on the (gateway) cluster.

| flow: ETS6.xml | | | default | |
|---|----------------------------------|-------------------------------------|---------------------|------------|
| mulation Parameters | Atopitoring [| | tglf_default | 🔾 Yes 🖲 No |
| Indiation Parameters Replet Execution | | | flags | |
| nitialisation Convergence Loop Pos | t_processing | | tglf_use_bper | 🔾 Yes 🖲 No |
| General Transport Equilibrium S | ources Transport Solver Edge | | tglf_use_bpar | 🔾 Yes 🖲 No |
| SpitzerModel | off | | tglf_adiabatic_elec | 🔾 Yes 🖲 No |
| SpitzerFrequency | every time step | | tglf_fastions | 🔾 Yes 🖲 No |
| SpitzerTimeIntervals | 0.0 | | tglf_dump_flag | 🔾 Yes 🖲 No |
| TurbulenceFrequency | every iteration | | tglf_calculate_angf | 🖲 Yes 🔾 No |
| TurbulenceTimeIntervals | 0.0 | | tglf alpha p | 1 |
| NeoclassicalModel | NCLASS | Code Parameters | tolf alpha e | 1 |
| NeoclassicalFrequency | every iteration | <u>×</u> | tglf alpha mach | 0 |
| NeoclassicalTimeIntervals | 0.0 | | talf alpha af | |
| DatabaseModel | 0# | Code Parameters | | 1 |
| DatabaseFrequency | every iteration | <u> </u> | tglf_alpha_quench | 0 |
| Database limeintervais | 0.0 | | tglf_xnu_factor | 1. |
| | Un Un | Code Parameters | tglf_sat_rule | 0 |
| AdditionalTimeIntervals | every iteration | <u> </u> | talf full wexb | 1 |
| Select_transport_combiner | TRANSPORT COMBINER | Code Parameters | tglf_nbasis_max | 4 |
| | | | tglf_nions | 0 |

The autoGui also allows parameter files be saved, shared and distributed between users - outside of training and developments work the autoGui is the recommended Frontend tool.



| Equlibrium | |
|----------------|--|
| Static | |
| Interpretative | |
| Chease | |
| Helena | |
| GKMHD | |

| Transport | |
|------------|--------|
| Database | MMM |
| Analytical | RITM |
| GLF23 | |
| Weiland | CDBM |
| EDWM | BgB |
| TGLF | Neowes |
| QLK | Neos |
| NCLASS | |
| NEO | |

| Sources | |
|-------------------|------------|
| Database | Cyrano |
| Analytical | Lion |
| BBNBI | Nbisim2 |
| Nemo | Risk |
| AFSI | Spot |
| Fusion_sources | Ascot4 |
| GRAY | StixRedist |
| GENRAY | FoPla |
| Torayfom | Pion |
| Torbeam | lccoup |
| runaway indicator | Impurities |
| Runaway fluid | Neutrals |

| Pedestal | Solvers | Edge |
|----------|-----------|---------|
| PENN | FEM | CEC |
| <u> </u> | Progronka | Solpsz1 |

In short: state of the art set of physics modules in a robust and highly configurable framework

A few models remains to be ported From ETSv5.





| Equlibrium | |
|----------------|--|
| Static | |
| Interpretative | |
| Chease | |
| Helena | |
| GKMHD | |

| Transport | |
|------------|--------|
| Database | MMM |
| Analytical | RITM |
| GLF23 | |
| Weiland | CDBM |
| EDWM | BgB |
| TGLF | Neowes |
| QLK | Neos |
| NCLASS | |
| NEO | |

| Sources | |
|-------------------|------------|
| Database | Cyrano |
| Analytical | Lion |
| BBNBI | Nbisim2 |
| Nemo | Risk |
| AFSI | Spot |
| Fusion_sources | Ascot4 |
| GRAY | StixRedist |
| GENRAY | FoPla |
| Torayfom | Pion |
| Torbeam | Iccoup |
| runaway indicator | Impurities |
| Runaway fluid | Neutrals |

| Pedestal | Solvers | Edge |
|----------|-----------|---------|
| PENN | FEM | CEC |
| | Progronka | Solpsz1 |

The range of modules available gives a user some flexbility to either "Zoom" to a specific physics aspect and/or vary fidelity from "scoping" to "advanced" through the selection of modules.



| Equlibrium | |
|----------------|--|
| Static | |
| Interpretative | |
| Chease | |
| Helena | |
| GKMHD | |

| Transport | |
|------------|--------|
| Database | MMM |
| Analytical | RITM |
| GLF23 | |
| Weiland | CDBM |
| EDWM | BgB |
| TGLF | Neowes |
| QLK | Neos |
| NCLASS | |
| NEO | |

| Sources | |
|-------------------|------------|
| Database | Cyrano |
| Analytical | Lion |
| BBNBI | Nbisim2 |
| Nemo | Risk |
| AFSI | Spot |
| Fusion_sources | Ascot4 |
| GRAY | StixRedist |
| GENRAY | FoPla |
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Some lingering general issues in relation to IMAS implementation: Where to store ML network data (files not allowed...) (Affects QLKNN; PENN)



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Fast lon physics is included in the equilibrium and the sources, restricted to dilution only in transport modules - largely by code owners recommendations.

Transport and H&CD well presented before will only discuss other and new aspects today.





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|----------|-----------|---------|
| PENN | FEM | CEC |
| <u> </u> | Progronka | Solpsz1 |

- ETS be used for both
- Interpretative and
- Predictive simulations!

Set up for JET; AUG, TCV; DEMO; MAST; ITER; WEST; JT-60SA as well as K-star and DIII-D



Bulk of the matter: Physics modules – the solvers



| - | |
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ETS has at its core a set of solvers that implements a comprehensive set of transport equations ("ASTRA-like") D. Kapulin 35th EPS, 2008 D. Coster, Trans. IEEE 2010

Solver implementation



Solvers directly imported from ETSv5.

- Progronka (Stankiewicz et al)
- FEM (Susnjara et al)
- Tested and verified
- Methods of Manufactured solutions (MoM)
- ITPA benchmarking \rightarrow

Pereverzev-Corrigan (CPC, 2008) stabilization scheme

- Required for stiff transport models
- Targetting steady state but usable for (slow) transients with strict time step control

Allowing for Internal Boundary condition r/a < 1

Rewritten equation set to allow for moving boundary



Advection-reaction-diffusion equations are very hard to solve for with stiff models in particular where the diffusivity not necessarily is dominant

Bulk of the matter: "Transients"





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|----------|-----------|---------|
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| | Progronka | Solpsz1 |

With stabilization schemes for stiff models activated, evolution is limited to (slowish) ramp-up/ramp down scenarios etc.

Current diffusion/ramp up





J. Ferreira WIMAS-2 team



Current diffusion/ramp up



Similar studies for ITER show similar performance (simple setup)



J. Ferreira WIMAS-2 team



AUG modeling in support of ECCD modelling for TAE stability analysis



q-profile is modified locally by ECCD. The increased magnetic shear has an direct impact on the TAE stability



Simulation done with ETS v6 (IMAS) using GRAY and CYRANO/StixReDist for ECCD and ICRH modeling respectively

J. Ferreira

Bulk of the matter: Impurities & Neutrals





| - | |
|----------------|--|
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| Chease | |
| Helena | |
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| Pedestal | Solvers | Edge |
|----------|-----------|---------|
| PENN | FEM | CEC |
| I | Progronka | Solpsz1 |

The impurity and neutrals modules are among the last to be moved to IMAS.

- Impurities already released

- Neutral package pending Impurities are now solved for as part of the general solvers

Impurities in ETS6 (implementation)



- Both interpretive/static and predictive evolution of the impurity densities is implemented
- Multiple impurities can be initialized 'from scratch' or read from the input IDSs
- Transport coefficients can be calculated by dedicated transport codes (NCLASS,EDWM,TGLF, QLK) or can be prescribed
 - Different ways of forming anomalous transport (per charge state, effective impurity species, or ignored)
- Source terms are obtained using latest version of ADAS database implemented through the AMNS library
- Difference from ETS5 implementation:
 - No longer a separate solver impurities integrated in main solver

D. Yadikin, I. Ivanova-Stanik, T. Johnson

Impurities in ETS6: verification





- Comparison with standalone SANCO (K. Kirov).
 - Based on JET #71827 (equilibrium), parabolic profiles, charge state bundles corresponding to boundary value 1.0e17m-3,
 - prescribed transport of 1.0m²/s is used, atomic data (ADAS, AMNS) sources
 - Run until steady state (flat profiles)

Impurities in ETS6: verification





- W results: discrepancy obtained using the latest version of the AMNS data (modified in Dec 2020) in ETS.
- Ni radiation: different atomic data used at JET, need further work to verify which version is 'correct'

Impurities in ETS6: verification





Pre december 2020 data

- W results: discrepancy obtained using the latest version of the AMNS data (modified in Dec 2020) in ETS. Understood! Fixed!
- Ni radiation: different atomic data used at JET, need further work to verify which version is 'correct'. Needs some further investigation!

Bulk of the matter: Pedestal predictions





| Equlibrium | |
|----------------|--|
| Static | |
| Interpretative | |
| Chease | |
| Helena | |
| GKMHD | |

| Transport | |
|------------|--------|
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| Pedestal | Solvers | Edge |
|-----------|-----------|---------|
| PENN | FEM | CEC |
| / | Progronka | Solpsz1 |

Pedestal predictions - PENN

- PENN Pedestal Neural Networks model
 - Estimates pedestal values from global/engineering parameters



• Database: EUROfusion JET pedestal database, provided by Lorenzo Frassinetti

- Size of training set: ~ 1500 entries (after dropping entries with missing values)
- We have data for electrons, not ions
- True values in database are used to optimize neural network through backpropagation

Training tools: Keras/Tensorflow interface, input and output normalization, minibatches

Andreas Gillgren

Pedestal predictions - PENN

Addressing Prediction Uncertainty: Simple bayesian approach:- train several neural networks to perform the same task

- The ensemble of predictions can be analysed to estimate uncertainty / detect extrapolation
- Ensemble networks may increase stability



Currently mainly based on JET data but broader adaptation to EUROfusion Pedestal dabatases underway. AUG data being assessed (however limited by AUG database size). Method obviously applies to synthetic data as well, EPED databases tec.

Andreas Gillgren

PENN in ETS

Generic Framework:

- 1. Training of neural networks is done before implementation (computational demanding part)
- 2. Parameters of optimized neural networks are exported to separate script/file
- 3. Python script on ETS to use neural network parameters and make rapid predictions (fortran based version planned)
- 4. Generic approach adapted to predictive modelling requirement in ETS



General implementation issue for all NN based models: how to deal with ensembles of network data in IMAS environments (e.g. how to avoid critical input files floating about at random - provenance capture, reusability, performance,.....) AMNS like library structure? Blessed file locations?



PENN in ETS

- Makes predictions from input IDS (IMAS framework) or CPOs (ITM framework)
- Writes new outer profiles (from boundary condition to LCFS)
- Uses modified tanh, requires 5 pedestal parameters (height, width, position, core slope, offset) to "extrapolate" to potential interior boundary point



- Non-static boundary conditions
- Predictive pedestals for predictive simulations

Work continues partially in and ENR and the intention is to provide model(s) (with better statistics) for all devices



PENN in **ETS**



JET shot 97781, Penn for pedestal (Gray area), TGLF for core, interpretatitve TRANSP

Comparison between INTERPRETIVE/TRANSP and PREDICTIVE ETS for 49.0 s -> 49.5 s



Jorge Ferreira

Core edge coupling



CEC -Core –edge coupling

Generic actor for passing data between core elements and edge codes.



Proof of principle use here but a very useful extension to bring in different edge modules - from simple analytical models to full blown edge codes.

D. Coster

DT extrapolations: fusion power





- General trend: less fusion power at larger minority fractions
- H min. case: Mainly dilution and smaller direct second harmonic acceleration of D+D_{nbi} ions (weaker bulk ion tails); *better performance at lower X[H]*
- ³He min. case: Dilution and smaller T+T_{nbi} acceleration, but maximum power achieved around $X[^{3}He]=2\%$ due to more efficient bulk ion heating

P. Huynh

JET modeling for DT extrapolation





Dominant ion (D+T) heating. External heating on D ions is larger than T ions; Central elec. heating due to ICRH (H min. + N=2 D acceleration)



from: Predictive simulations with ETS including NBI/ICRH Synergy for baseline shot 92436, P. Huynh, E. Lerche, D.Van Eester, JET TEAM and WPCD TEAM, JET TF Meeting

References:

P. Hyunh, *et al.*, European Transport Simulator modelling: Modelling of the role of ICRH/NBI synergy in the DT extrapolation of high-power JET D scenarios to D-T, accepted for publication in Nuclear Fusion P.Huyn, *et al.*, Modeling ICRH and ICRH-NBI synergy in high power JET scenarios using European transport simulator (ETS), AIP Conference Proceedings 2254, 060003 (2020); https://doi.org/10.1063/5.0014240

Fusion power prediction with the reference discharges (#96994 and #97781) in DTE2





- DT equivalent fusion power (i.e. no increase in T_i and n_i profiles due to positive isotopic effect and high heating)
 = 9 ~ 10MW in both baseline and hybrid
- Predicted DT fusion power with predicted T_i and n_i profiles
 - DT simulation with 33MW heating: 8~10.5MW in baseline and 10~12MW in hybrid.
 - DT simulation with 40MW heating: 12~16MW in baseline and 13~17.5MW in hybrid.

Hyun-Tae Kim, on behalf of T17-07 modellers | Task Force meeting | Zoom conference | December 2020 | Page 22

T17-07 modelling is progressing and this is likely not the current state of affairs

Edge turbulence WF with synthetic diagnostics





Turbulence WPCD workflows including synthetic diagnostics to compare modelled data of SOL filamentary transport to experimental data in collaboration with WPMST1 and WPJET1.

Linear MHD stability chain for energetic particles and non-linear codes for fast-ion MHD interaction

- Updates to HYMAGYC now includes, among others, the possibility to load a Energetic Particle population accordingly to the parametrised distribution function fitted from H&CD modelling codes.
 - It runs as a parallel actor both using a fortran "driver" and a test Workflow.
- The hybrid drift-kinetic code CASTOR-K has been adapted to use IDSs. A driver code also exists to enable the running of the code offline, cast as an element of a dedicated workflow.
- A new fitting tool called STARFISH has been implemented to perform the global fit of the numerically obtained energetic particles distribution functions using a parametric Equilibrium Distribution Function (EDF) in term of constants of motion, w (kinetic energy per unit mass), λ=µ/w (the generalized pitch angle), P_φ (the canonical toroidal momentum).
 - The implementation is now fully integrated with the Kepler Environment and with the ITER Integrated Modelling and Analysis (IMAS) framework.
 - The STARFISH project has been created on the WPCD GFORGE repository and a first tag for the STARFISH suite of fitting tools has been released.

Linear MHD stability chain for energetic particles and non-linear codes for fast-ion MHD interaction





A MATLAB code has been implemented to perform the best fit of the parametrized EDF solving a bound-constraint global optimization problem. A custom Genetic Algorithm (GA) has been implemented to perform a population-based elitist global search in 6D parameter space and in cascade (GENiE toolbox), if selected by the end-user, a local search can be performed by means of state-of-the-art local optimizers. The implementation is integrated with the Kepler Environment and with the ITER Integrated Modelling and Analysis (IMAS) framework.

Summary



WPCD (and ITM-TF) created the philosophy, prototyped and structured the infrastructure (ISP/CPT) and paved the way or IMAS.

The intended continuation into the new e-tasc structured largely failed leaving gaps in implementation, several alienated or unsupported model developers – however

A core set of tools remains (ETS; EQSTAB; EQRECONSTRUCT;...) with an active (and hopefully) expanding user community that is managed through a small ACH activity.





CD-IO meeting