TRANSP User's Group meeting, March 23-24 2015, PPPL, US

EUROfusion

EUROfusion effort in code development for integrated modelling

Presented by Irina Voitsekhovitch on behalf of WPCD and WPISA

WPCD Project Leader: Gloria Falchetto

PMU WPCD and WPISA RO: Irina Voitsekhovitch

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Contributions to this talk:

G. Falchetto, X. Litaudon, R. Coelho, D. Coster, T. Johnson, P. Strand, O. Asunta, C. Atanasiu, V. Basiuk, R. Bilato, Yu. Baranov, D. Farina, J. Ferreira, L. Figini, A. Figueiredo, K. Gal, R. Hatzky, O. Hoenen, P. Huynh, F. Imbeaux, I. Ivanova-Stanik, D. Kalupin, F. Koechl, E. Lerche, A. Merle, S. Nowak, M. Owsiak, T. Ribeiro, D. Samaddar, O. Sauter, M. Schneider, D. Tskhakaya, D. Van Eester, WPCD and WPISA teams

Outline

- Place and role of Work Packages Code Development (WPCD) and Infrastructure Support Activities (WPISA) within EUROfusion
- WPISA: integrated modelling framework, infrastructure and support activities
- WPCD: Code Development for Integrated Modelling (IM)
  ongoing workflow developments:
  - *equilibrium and MHD stability chain*
  - *core transport simulator: the ETS*
  - *heating and current drive*
  - *edge codes*
- Outlook and prospects
- Liaison with international projects (ITER, ITPA), contributions to DEMO modelling
- Discussion: TRANSP role and position in the EU Integrated Modelling

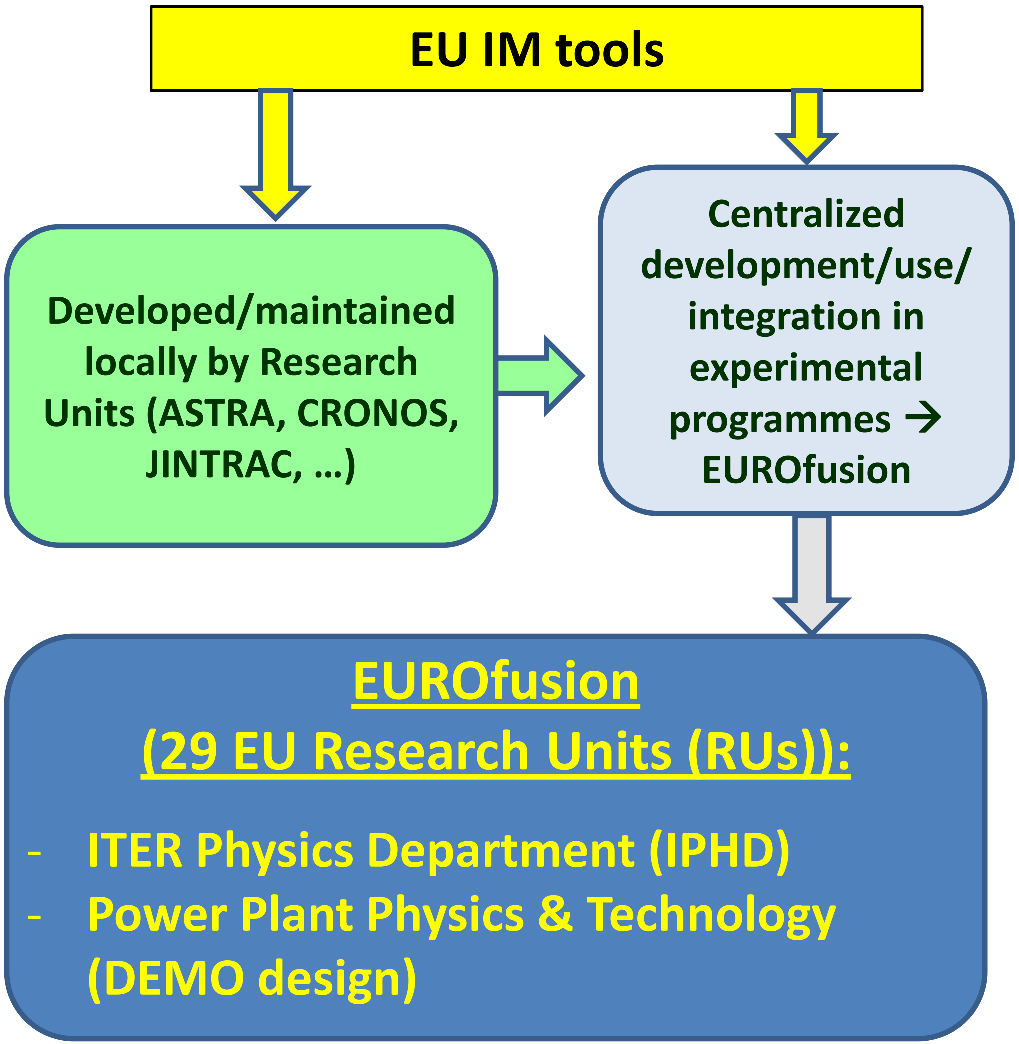
Fusion Roadmap - a strategic vision to demonstrate the generation of electric power by DEMO by 2050: importance of IM

Identified integrated modelling (IM) priorities:

- ***Building confidence in the predictive capability of IM tools*** *- V&V involving a broad range of expertises over a range of devices (conventional and spherical tokamaks, stellarators)*

- ***Broad access and use of a centrally maintained suite of IM tools*** *as a production level facility and a test bed for new developments → the supporting code integration framework and computational resources*

- ***Supporting the development of modular sets of codes and modules covering a range of physics areas*** *– the transition from research to production level codes (robustness, performance)*



Place and role of Work Packages Code Development (WPCD) and Infrastructure Support Activities (WPISA) within EUROfusion

ITER Physics Department

Physics programmatic structure:

- **Mission 1: Plasma Regimes of Operation** (*ELMs, runaways, disruptions, MHD, fast particles, plasma control, …*)
- **Mission 2: Heat Exhaust System** (*detachment control, PFC, divertor/SOL modelling, …*)
- **Mission 8: Stellarator** (*qualification of Helias optimised stellarator operation, theory and modelling,…*)

Implementing Work Packages:

- JET1-JET4
- MST1, MST2
- PFC
- DTT1, DTT2
- S1, S2
- SA (JT60SA)
- CD
- ISA

WPCD: Integrated Modelling tools to be provided for modelling support to all IPHD missions

WPISA: integrated modelling framework, support to users and developers, code optimisation

Experimental work packages: use of IM tools for analysis and modelling of existing experiments, planning for future experiments → joint experimental-modelling teams

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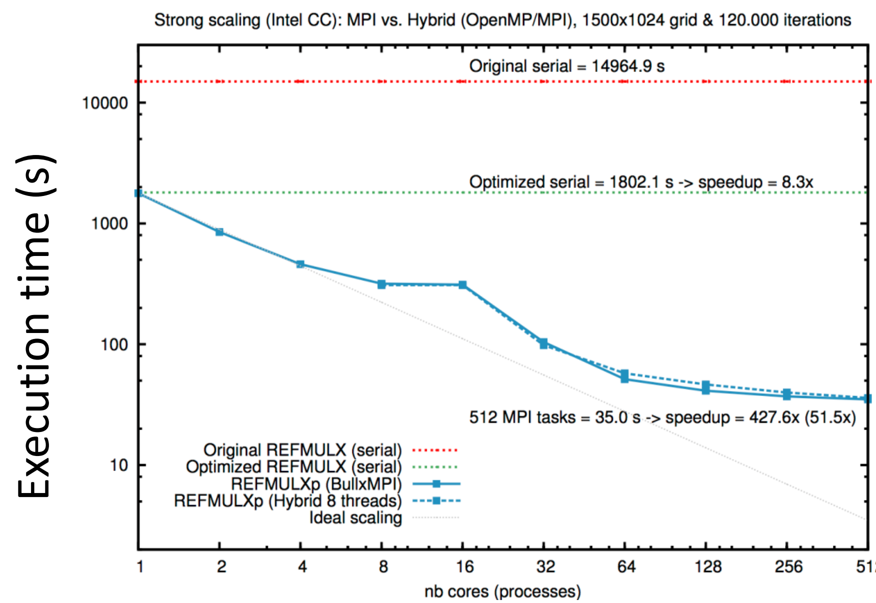
Work Package Infrastructure and Support Activities (WPISA)

- **Core Programming Team** (CPT, F. Imbeaux): IT experts (5.5 ppy) providing support to IPHD modelling programme
- **Gateway team** (D. Coster): a dedicated cluster with a centralized installation of the infrastructure
- **High Level Support Team** (HLST, R. Hatzky) - experts in code parallelisation (8 ppy):
  - *Optimisation and parallelisation of EU codes (Open MP and/or MPI standards for massively parallel computers)*
  - *Support to WPCD*
  - *Exploration of alternative frameworks:*

    - Integrated Plasma Simulator (IPS): tackle workflows making extensive use of HPC resources

    - ADIOS (US developed): robust technology for large HPC jobs checkpoint / restart

Optimisation of REFMULX (x-mode reflectometry): maximum speedup factor of ~430 is achieved compared to original non-optimised serial code



[T. Ribeiro, Filipe da Silva, private communication "Parallelization of the X-mode reflectometry full-wave code REFMULX", 28th October 2014, Department of Computational Plasma Physics, IPP, Garching, Germany]

EU integrated modelling framework

- The EU IM approach: use of a standardized data-structure, independent of workflow technology:
  - ✓ generic data and communication ontology
  - ✓ CPOs: Consistent Physical Objects [F. Imbeaux, Comp. Phys. Commun., 2010]
  - ✓ both plasma physics and technology data included (simulated and experimental)
- Centralized platform & software infrastructure on a dedicated Gateway
  - ✓ modular
  - ✓ flexible
  - ✓ machine general
  - ✓ language independent (Universal Access Layer)
- Currently using Kepler workflow manager
  - ✓ Allows to easily build new workflows
  - ✓ Enables mixed language programming
  - ✓ Allows to execute parts of a workflow from a Kepler session running on 1 node on the Gateway as:
    - ✓ batch queues on the Gateway cluster
    - ✓ batch jobs on an external HPC
    - ✓ use GRID resources

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Work Package: Code Development for Integrated Modelling

Development of existing modelling codes with a particular focus on integrated modelling:

- provide a suite of codes that can be validated on existing machines and used for ITER and DEMO predictions
  - **build on** existing modelling codes including the EU-IM **infrastructure, toolset and codes developed under the EFDA ITM Taskforce**
  - **add new physics to the existing models**
  - couple codes into **integrated workf**lows
  - **code optimisation**

- specific ITER simulation work in support of ITER IO and F4E with specified deliverables

CD Project structure

- **Code Development for Integrated Modelling Project**
  - **ACT1- Equilibrium and stability chain development and exploitation**
  - ACT2- Free Boundary Equilibrium + control workflows
  - **ACT3- Core transport simulator**
  - ACT4- Turbuence workflows with synthetic diagnostics
  - **ACT5- Heating and current drive workflow**
  - ACT6-Benchmarking of non-linear codes for fast-ion and MHD interaction
  - **ACT7-Edge/SOL code development**
    - **SOLPS technical optimization**
    - AMNS data and interfaces
    - **edge/SOL code implementation and workflow development**
    - core/edge and edge code adaptation
  - ACT8- Support activities
    - portal /webpage maintenance
    - visualization tools development
    - experimental data interface
    - synthetic diagnostics
  - ACT9 - 3D code for halo current formation (JOREK-STARWALL)

Linear MHD stability workflow (EQSTABIL)

- Reconstructed equilibrium → high resolution equilibrium → MHD stability

Courtesy R. Coelho

DDF Director

Welcome to the EQSTABIL workflow !
Present version features :
- start from an itmdb cocos=13 free bnd reconstructed equilibrium or fixed bnd equilibrium (single slice)
- cut-off equilibrium (if free bnd reconstructed) and refine it with HELENA, CHEASE or CAXE
- calculate the linear stability with ILSA, MARSGW/MARSF or KINX
- visualize/save eigenfunctions

- shot: 77877
- run_in: 2
- run_out: 998
- run_work: 999

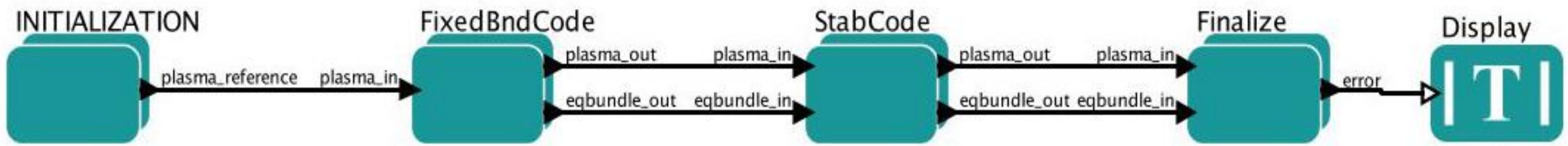
- device: jet
- user: rcoelho

- eqcode: helena
- stabcode: marsgw
- cut_eq: no

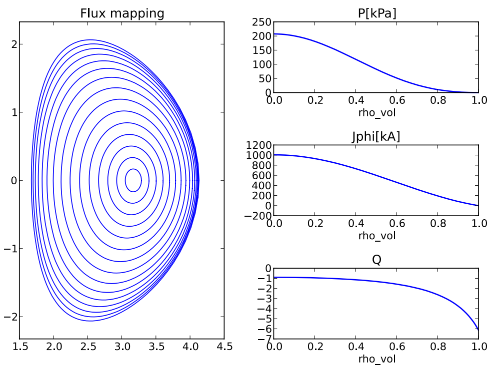
→ Can be used for ANY device/shot, as a stand-alone WF and to be plugged into any workflow

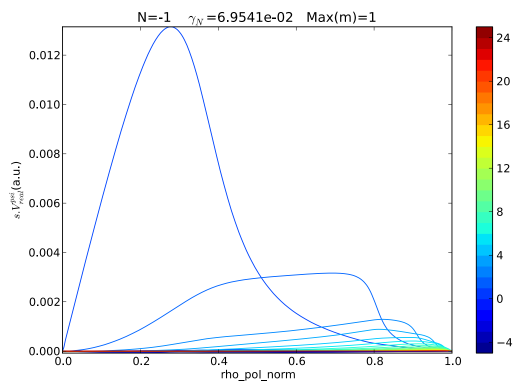
→ equilibrium interchangeability (HELENA→CHEASE): sensitivity of MHD growth rates to equilibrium

Test case: JET n=1 internal kink



Input:
- fixed boundary
- plasma profiles





New task 2015: integration of error bars on equilibrium and confidence analysis

J - alpha Kepler workflow application

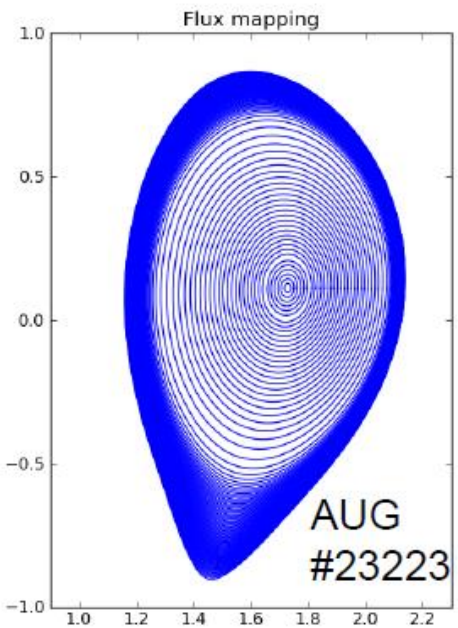
High refined equilibrium → JALPHA modify → edge MHD stability

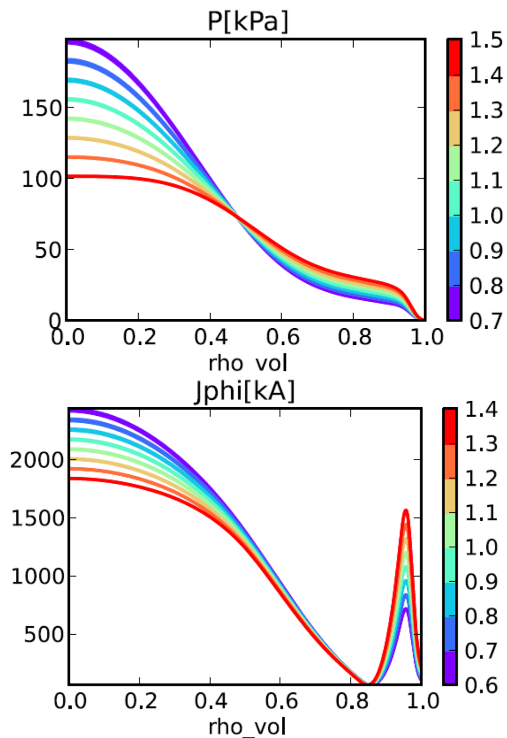
Courtesy R. Coelho

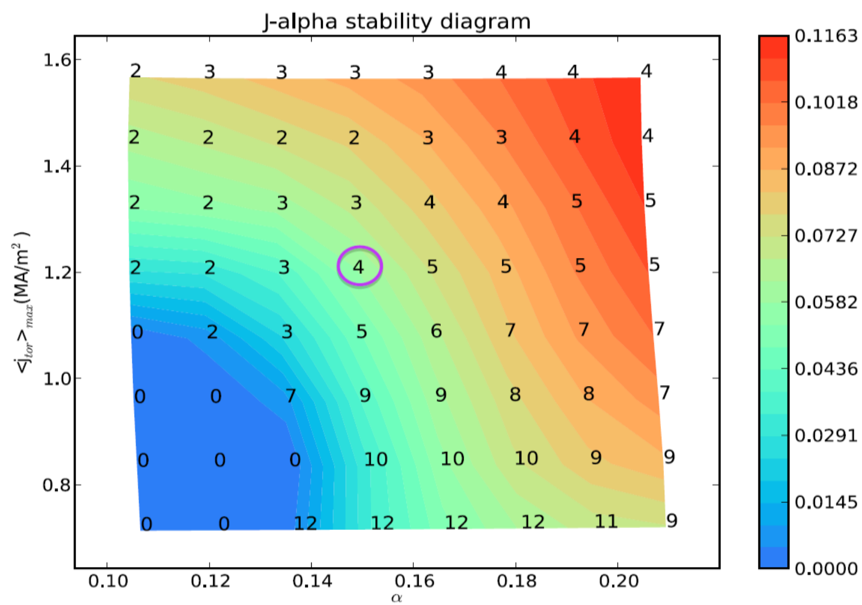
Workflow operates as a user interface:

- choice of input equilibrium;
- configure the pedestal pressure/current scaling coefficient scan;
- configure the linear MHD scan in toroidal mode number e.g. n-range, poloidal harmonics
- visualization of the results

AUG edge stability test case (#23223) (equilibrium: high resolution CLISTE run with kinetic constrains)







State-of-the-art EU transport simulator: ETS

- 150 composite actors
- interchangeability of modules with different physics sophistication

EQUILIBRIUM:
Fixed : BDSEQ, EMEQ, SPIDER, HELENA, CHEASE
FBE: CEDRES++, FREEBIE

TRANSPORT:
Interpretative
Predictive anomalous: ETB (analytical), BgB (empirical), Weiland, GLF23, EDWM, RITM, MMM (theory-based)
TGLF (serial) Qualikiz
Predictive neoclassical: NEOS, NEOWES, NEOART, NCLASS/FORCEBAL
Coupling to turbulence code: GEM

IMPURITIES (all ionization states)

MHD
NTM
SAWTEETH
ELMs

Position Control

ETS
1.5D Core Transport Solver

SOLPS

ERO

Power controls

HCD - sources:
ECRH/runaway: GRAY, *TRAVIS*, LUKE/C3PO*
ICRH waves: LION*, TORIC*, CYRANO, EVE
NBI : *BBNBI**; NEMO
Ion Fokker Planck : *ASCOT*, SPOT**, RISK,
PION (incl. IC/NB/alpha synergies)
El. Fokker-Planck: RELAX
nuclear sources: *nuclearsim*, DRESS*

PELLETS

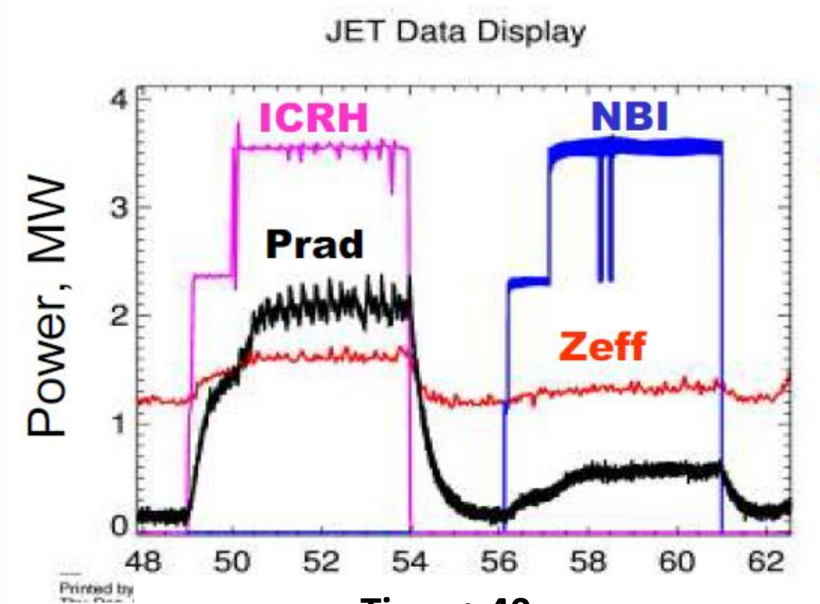
NEUTRALS (fluid)

pellet frequency control

Color code
ready
under testing
planned in 2015

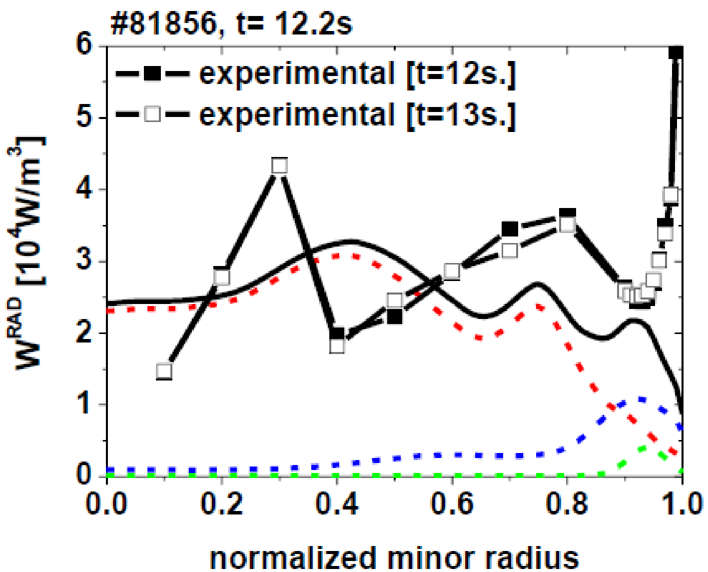
suitable for stellarator *very detailed physics time demanding

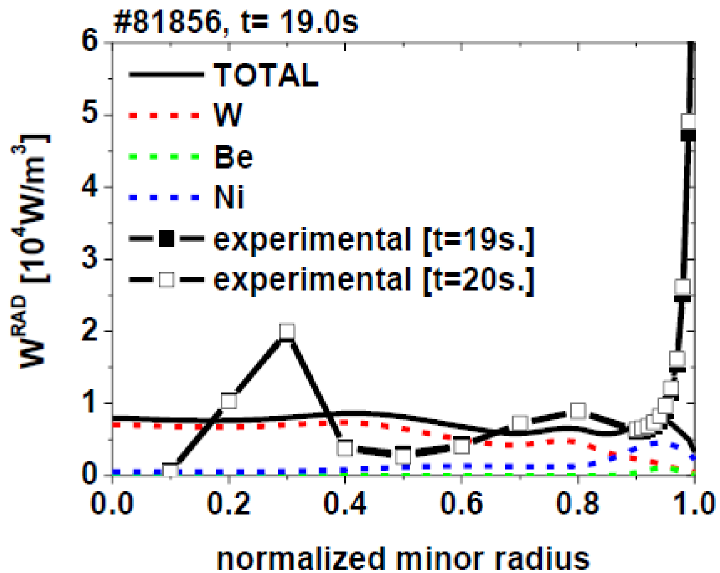
Core impurity simulations with ETS: ILW, L-mode



Time + 40 s

I. Ivanova-Stanik, D. Kalupin, J. Ferreira





- Impurity (Be, Ni, W) simulations with measured ne and Te. Bohm-gyroBohm transport for impurities, zero convection. ADAS cross-sections.

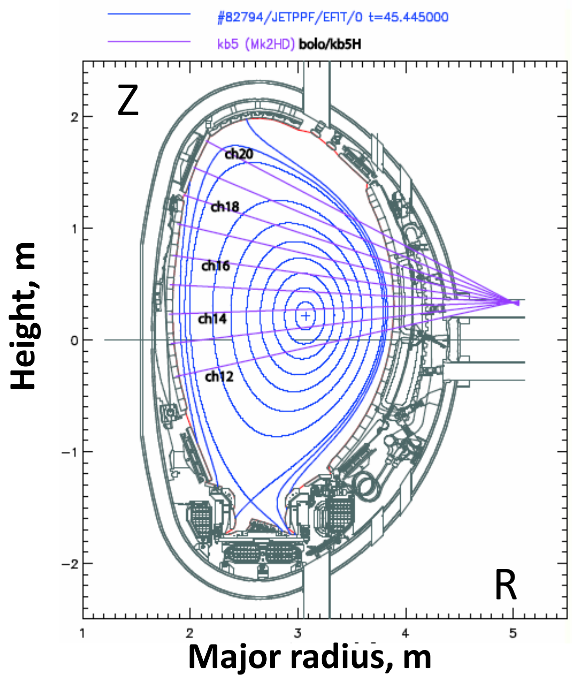
- Boundary conditions: nNi (measured), nW (to match Prad), nBe (to match Zeff). Coronal equilibrium for bndry and initial charge states.

- Simulated total Prad shape and Ni radiation is found to be consistent with measurements.

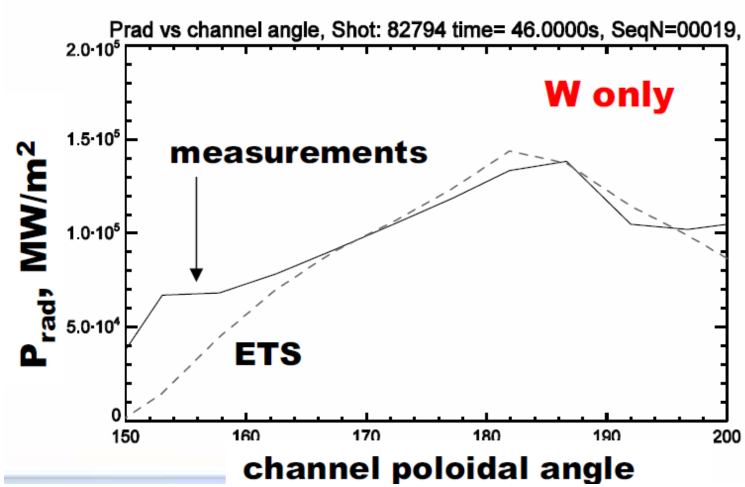
- Core radiation is dominated by W while Ni provides edge radiation. Zeff is mainly determined by Be

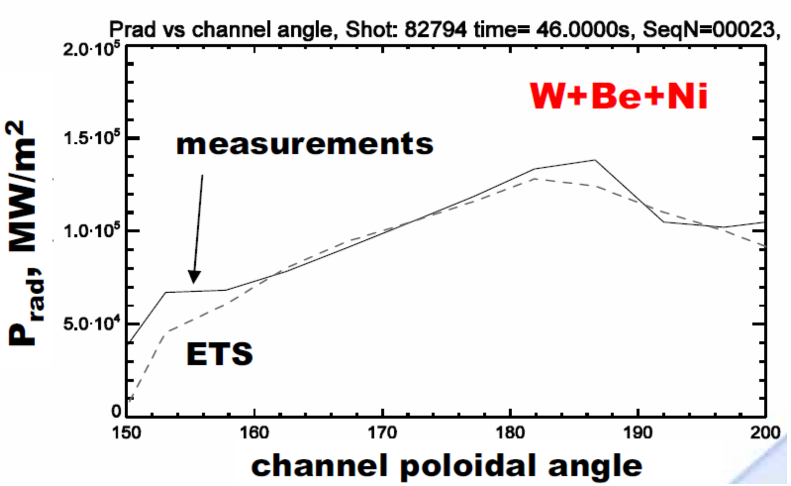
Core impurity simulations with ETS: ILW hybrid scenario

- Impurity densities (W, Be, Ni) are simulated using measured electron density and temperature
- Impurity transport ($D_{imp}=2D_{BgB}$ + 2.5 m^2/s, V_W=5 m/s, V_{Be}=3.5 m/s, V_{Ni}=4 m/s) and boundary densities are adjusted to match total P_{rad}, central line averaged Z_{eff} and Ni concentration
- Radiation along the bolometer lines of sight is simulated



I. Ivanova-Stanik, Yu. Baranov

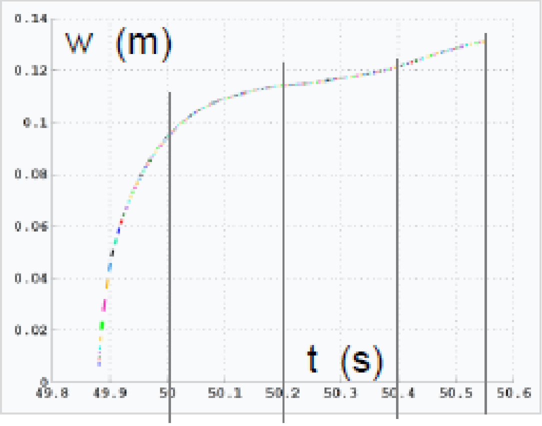


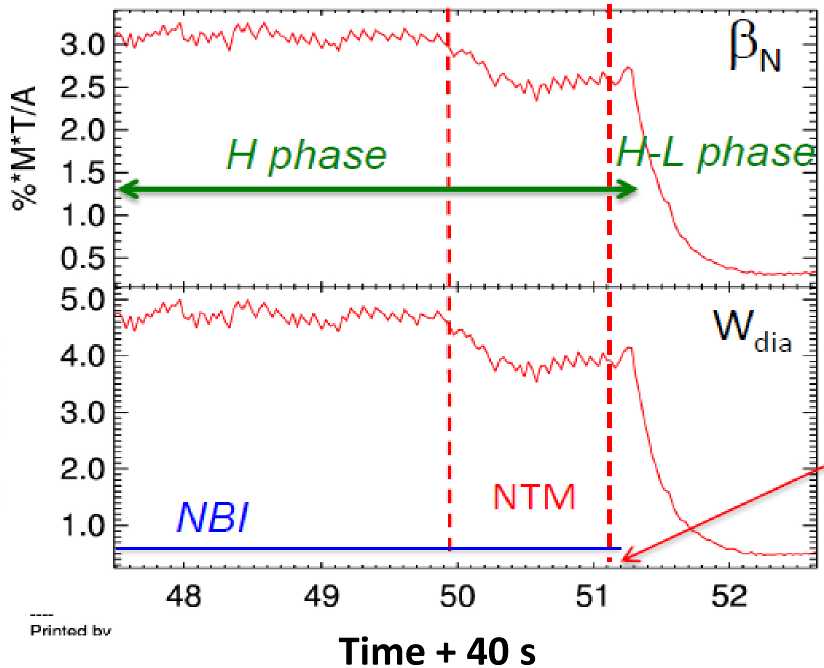


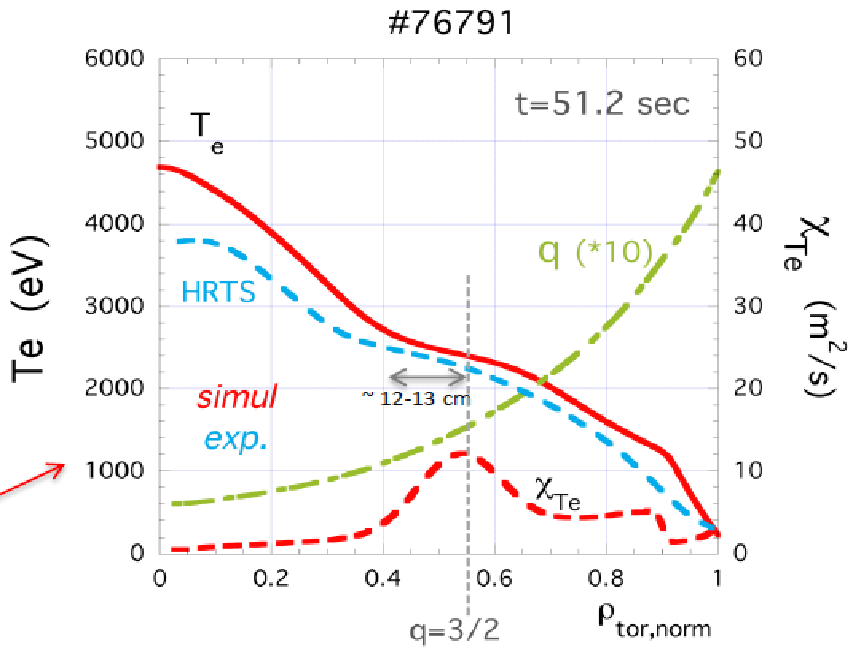
NTM driven transport

S. Nowak, O. Sauter, V. Basiuk, P. Huynh, A. Merle

- equilibrium (CHEASE) and current diffusion are simulated
- T_e, n_e, T_i profiles simulated using the BgB transport enhanced by NTM (when unstable), KIAUTO for pedestal simulations
- island width simulated self-consistently with temperature and density
- full discharge simulations (Ipl rampup→rampdown) are performed for this shot



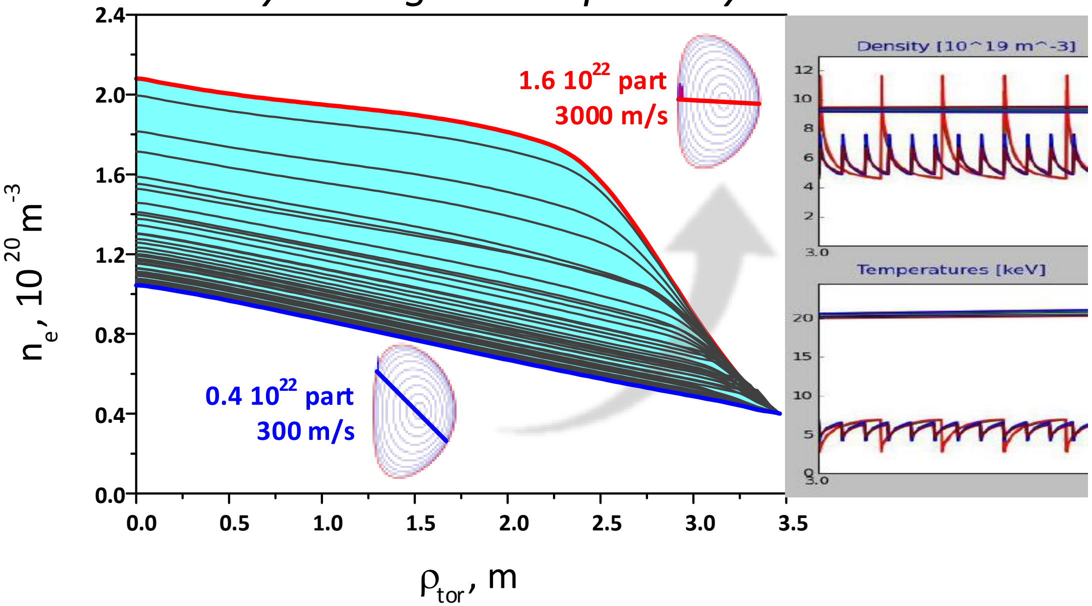


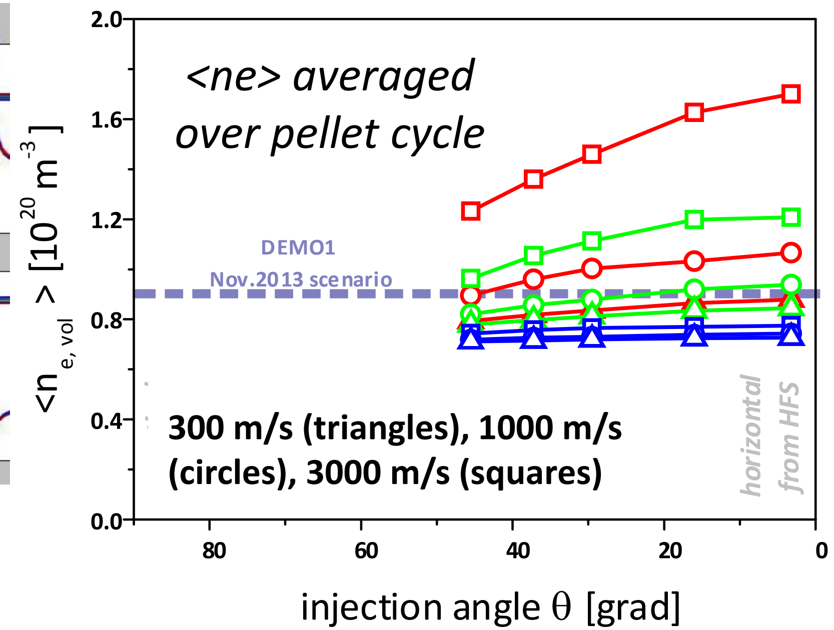


Pellet modelling (optimisation of fuelling in DEMO)

Density averaged over pellet cycle

D. Kalupin, R. Coelho, M. Owsiak, O. Hoenen



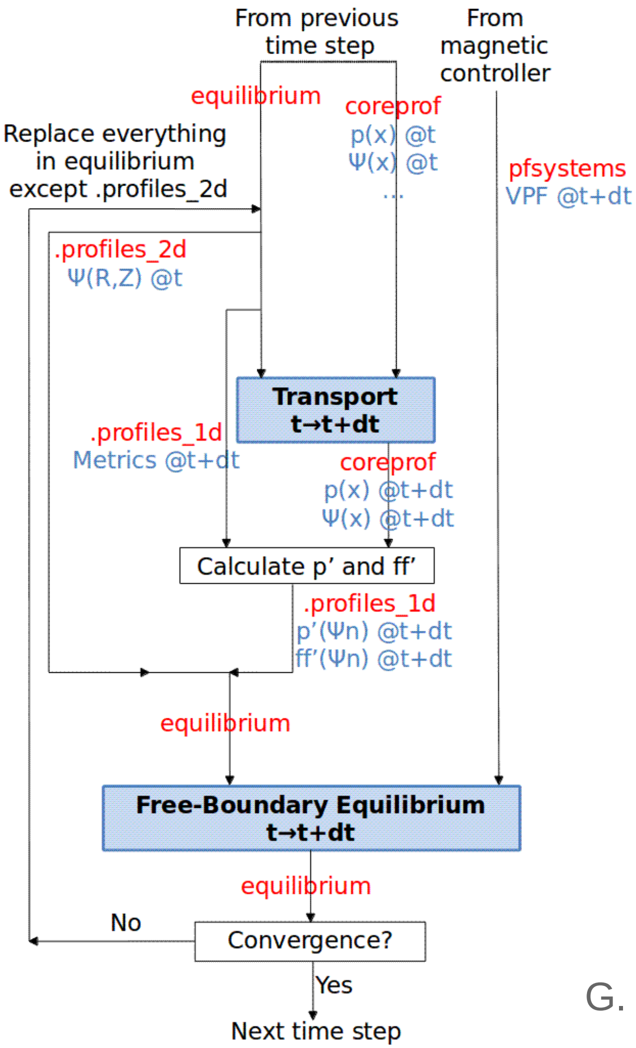


- **Pellet model composed of two parts:**
  - ***Ablation*** *– The erosion rate of the pellet*
    - Deuterium [K Gal et al, NF 2008]
    - *Other species – less complex [B.V. Kuteev, NF 1995]*
  - ***Deposition*** *– Mass relocation of the ablated material due to drift effects [http://www.euro-fusionscipub.org/wp-content/uploads/2014/11/EFDP12057.pdf)]*
- **ETS simulations (Te, Ti, ne, nimp, j) to match global DEMO parameters estimated by PROCESS**
- **Frequency compensates for the size of pellet: same throughput in all runs**

→ **The velocity and size of pellets are optimised to produce high density plasma**

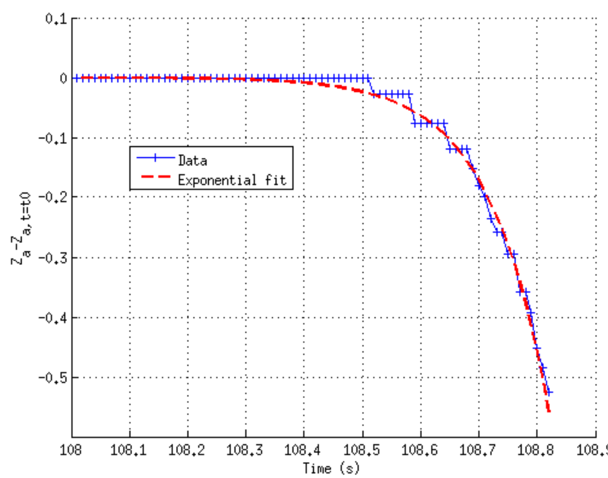
Free boundary ETS simulation

A switch in ETS workflow allows to select a FBE solver in place of the fixed-boundary solver.



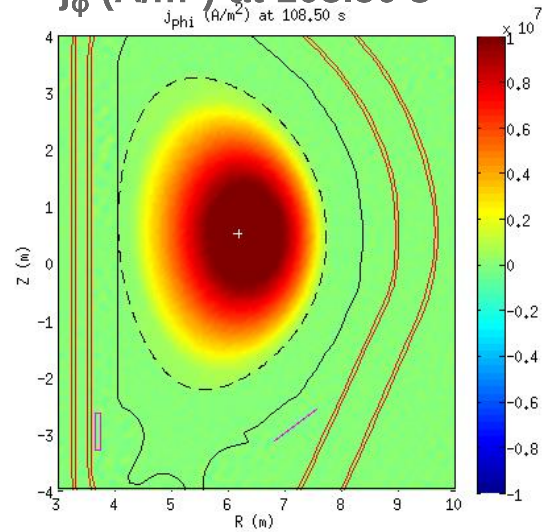
Simulation of a VDE in ITER.

The initial plasma has I_p=11.8 MA, elongation κ=1.49, limited on the HFS. PF voltages are set to 0.

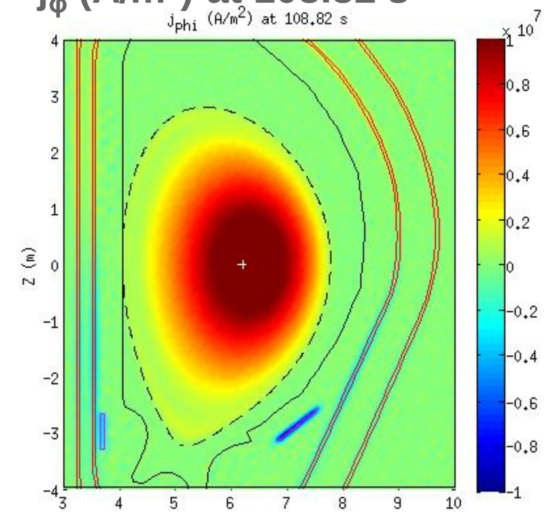


G. Falchetto et al. Nucl. Fusion 2014

j_φ (A/m²) at 108.50 s



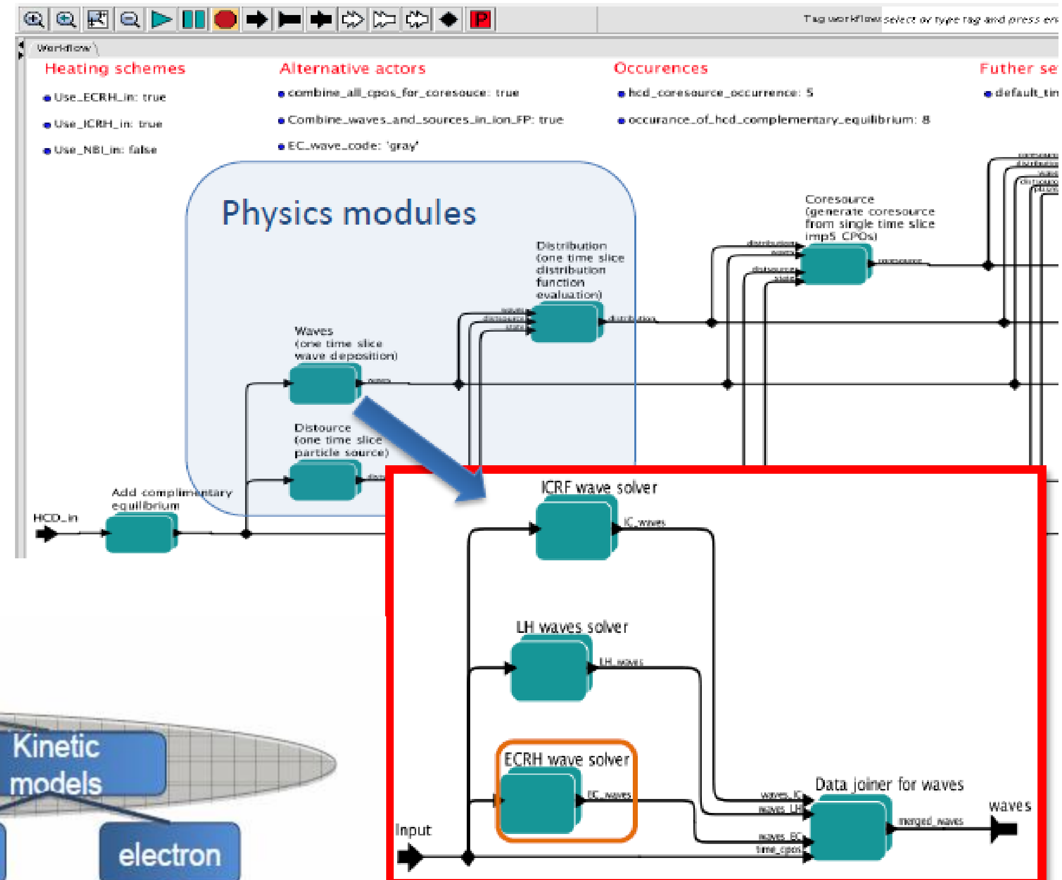
j_φ (A/m²) at 108.82 s

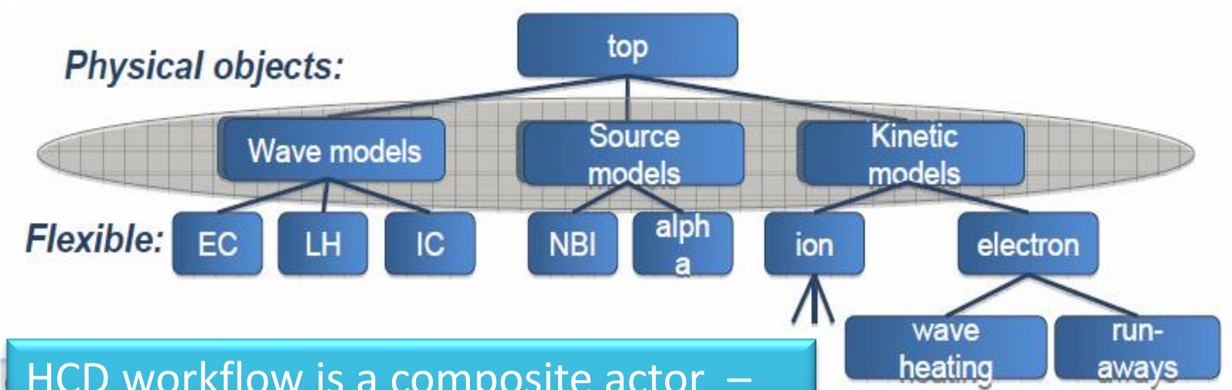


Heating and Current Drive

The HCD-Workflow: EC, IC, NBI, alpha-heating

- ***Physics:** wave propagation, diffusion and absorption, plasma-wave interaction, beam slowing down, atomic processes, synergy between heating schemes*
- ***Implementation:** modules based on physics options (not heating schemes)*





HCD workflow is a composite actor – to be plugged into any workflow, as ETS, or can be used as stand-alone

courtesy T. Johnson

ECRH benchmark

L. Figini et al, 17th Joint Workshop on Electron Cyclotron Emission and Electron Cyclotron Resonance Heating, 2012

- Standard inductive ITER H-mode scenario
- Various EC configurations: UL and EL
- Codes are interchangeable within the same workflow

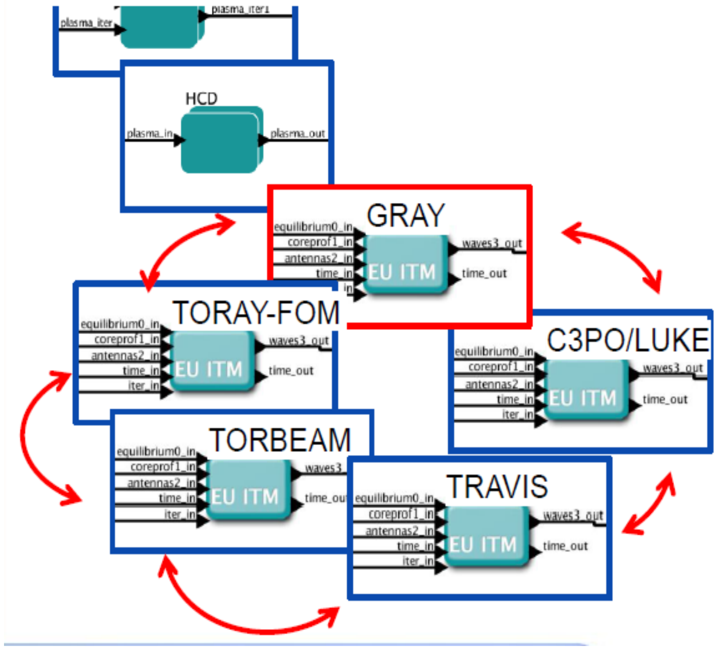
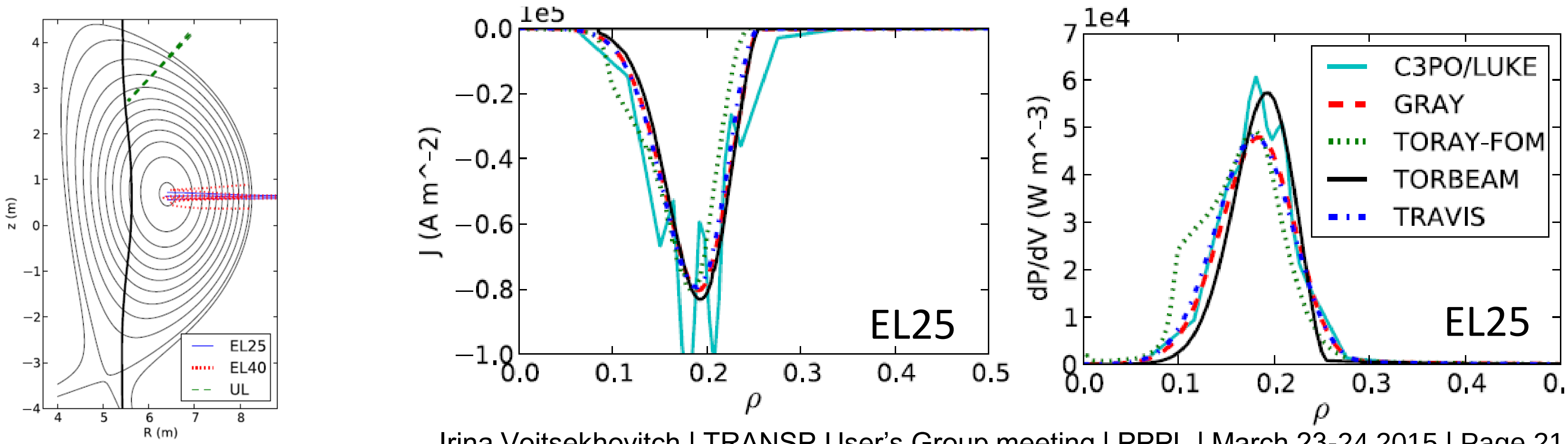


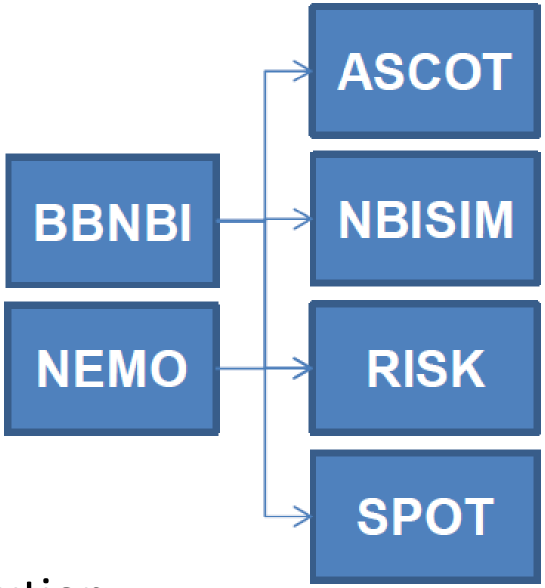
Table 1. Summary of the main features of the codes involved in the benchmark.

Code name	Propagation model	Boundary model	Absorption model	Current drive model
C3PO/LUKE	multi-ray, cold/ warm dispersion	Snell's law	bounce-averaged relativistic Fokker-Planck, linear/quasi-linear	
GRAY	quasi-optical rays, cold dispersion	polynomial SOL	analytic, relativistic/ weakly relativistic	adjoint, HS limit/ momentum conservation
TORAY-FOM	multi-ray, cold/ warm dispersion	unlimited SOL	analytic, relativistic	adjoint, HS limit/ momentum conservation
TORBEAM	Gaussian beam, cold dispersion	Snell's law	analytic, relativistic/ weakly relativistic	adjoint, HS limit/ momentum conservation
TRAVIS	multi-ray, cold/ warm dispersion	Snell's law	analytic, relativistic	adjoint, momentum conservation



Ongoing NBI benchmark (preliminary results)

8 various combinations

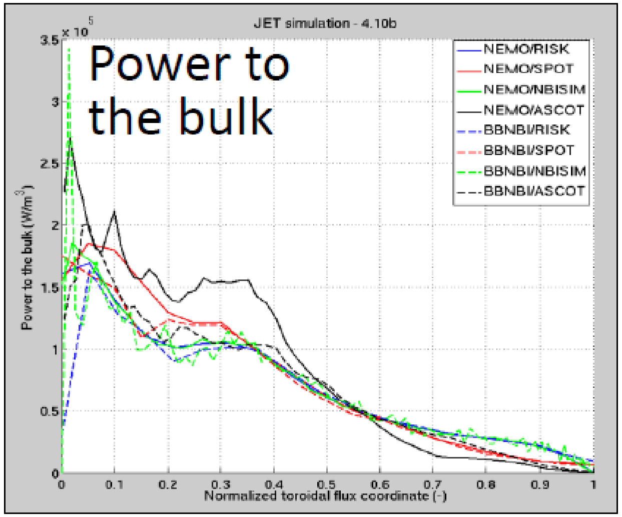


NBI and alpha-particles:

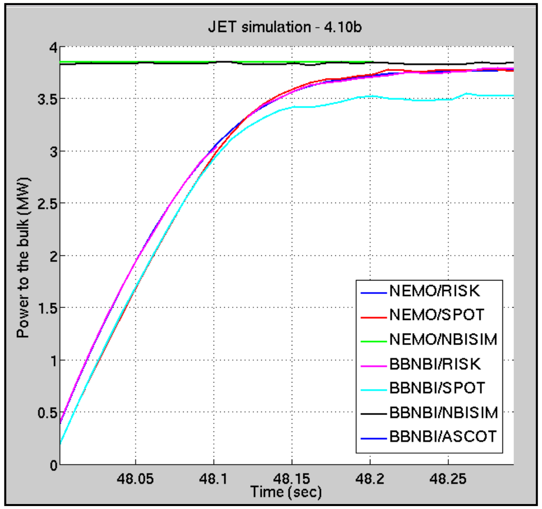
- **Beam deposition**: **BBNBI, NEMO**
- **Simulations of nuclear reactions using beam deposition**
- **Fokker-Planck** (fast-ion slowing down): **ASCOT, SPOT, Risk**

Benchmarks on all possible combinations are ongoing [M. Schneider et al, EPS 2015]

JET #77922



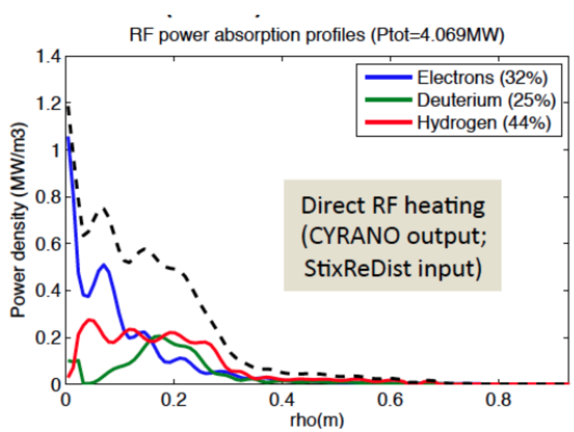
Power; time evolution

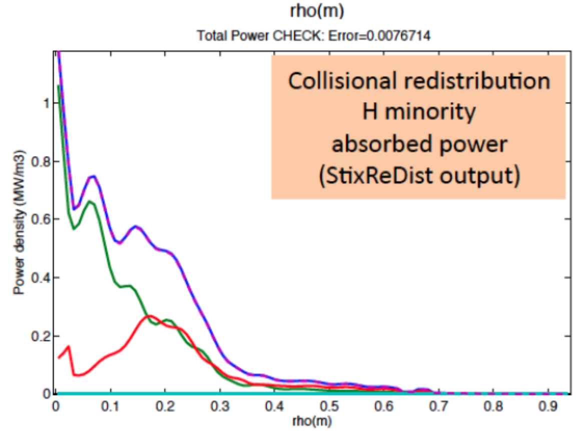


Status of ICRH codes

- **waves field solvers:** CYRANO, EVE, LION, TORIC
- **Fokker-Planck** (fast-ion slowing down): SPOT, StixReDist (ASCOT being ported)
- **benchmarking in progress** [R. Bilato et al, AIP Conf. Proc. 1580, 291, 2014]

courtesy D. Van Eester & E. Lerche





Coupling Cyrano/StixReDist within the HCD workflow:

- *CYRANO* [E. Lerche et al, PPCF 2009]: 2D full-wave coupled full wave, RF dielectric response of plasma species with general (i.e. non-Maxwellian, not in WPCD yet) particle distribution

- *StixReDist* [D. Van Eester and E. Lerche, PPCF 2011]: 1D (isotropic) QLFP code (Stix/Karney's formalism), fundamental and 2nd harmonic ICRH minority and majority species. Separate actor. Next step – RF accelerated beam ions

EDGE codes within WPCD

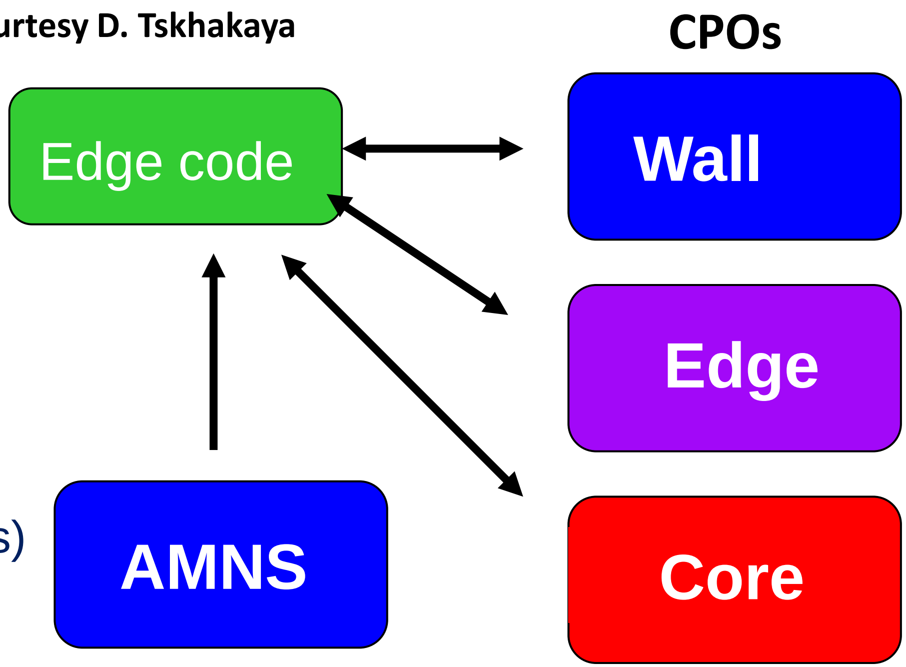
Edge codes using CPOs:

- ✓ **BIT1** (1D SOL, fluid plasma, neutral, impurities)
- ✓ **ERO** (3D MC impurity test particle approach)
- ✓ **SOLPS** (2D Braginski eqs, impurities)

Ongoing adaptation:

- ➢ **COREDIV** (1D core+slab 2D SOL, impurities)
- ➢ **TECXY** (2D fluid (main plasma, neutrals), divertor geometry, drifts)

courtesy D. Tskhakaya



Core-edge integration:

- *ETS-SOLPS coupling done in Fortran [G. Falchetto et al, NF 2014], coupling in Kepler in progress*
- *COREDIV is ported to Gateway*

Wall CPO: wall surface material, temperature, …

Edge CPO: physics, space grid type description

Core CPOs: plasma profiles, equilibrium, fluxes

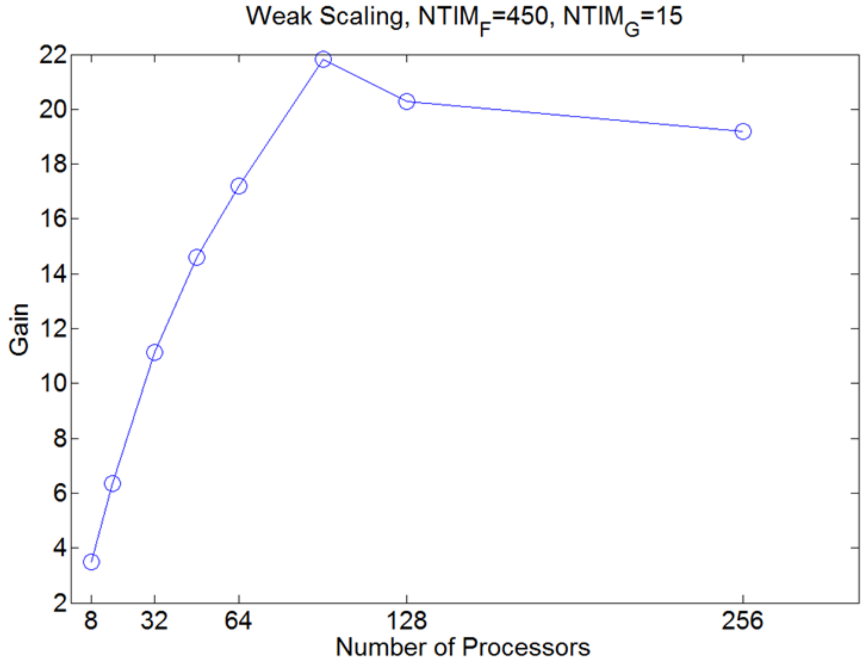
AMNS CPO: collision CS, rates, particle release yields

See talk by Sven Wiesen

SOLPS technical optimization outcomes

D. Samaddar

- **Parareal: speed-up > x10** on 100 – 256 cores
  - more realistic test cases in 2015:
    - ITER case with ELMS (B2 only)
    - B2-EIRENE with drifts



- **OpenMP parallelization of B2** (**EUFORIA+HLST+RZG)**
  - **x6 speed-up** on 10–20 cores for an ITER case with large number of charge states
  - coupling of OpenMP B2 with MPI EIRENE is ongoing

Outline

- Place and role of Work Packages Code Development (WPCD) and Infrastructure Support Activities (WPISA) within EUROfusion
- WPISA: integrated modelling framework, infrastructure and support activities
- WPCD: Code Development for Integrated Modelling (IM) ongoing workflow developments :
  - *equilibrium and MHD stability chain*
  - *core transport simulator: the ETS*
  - *heating and current drive*
  - *edge codes*
- Outlook and prospects
- Liaison with international projects (ITER, ITPA), contributions to DEMO modelling
- Discussion: TRANSP role and position in the EU Integrated Modelling

ETS with improved capabilities

- Implementation of **ELM module**
- Integration of **quasilinear anomalous transport modules** (Qualikiz, TGLF)
- Development & implementation of **heating synergies (IC, NBI, α sources)**
- Update of HCD workflow including synergies & **runaway electron** module
- **Integration of a controller** and **test of feedback controlled ETS workflow on ITER/JET cases**
- **First ETS release to users**: installation on JET analysis cluster, development of data access routines and implementation of data consistency diagnostics for benchmarking against TRANSP

Link to EU experiments
Interpretative analysis and modelling of select JET discharges with ETS
Validation of the ETS with free boundary equilibrium
ETS particle transport analysis of JET and MST discharges
ETS scenario modelling for DT campaign fuelling: start to assess tools for DT modelling beyond present transport codes capabilities

Other ongoing workflow developments

- ***RWM workflow***
- ***Development of prototype Kepler workflows for core-edge coupling and edge workflow modelling SOL and interaction with PFCs***
- ***Application of workflows coupling a edge/SOL turbulence code to probe/ reflectometry synthetic diagnostics to experiments***

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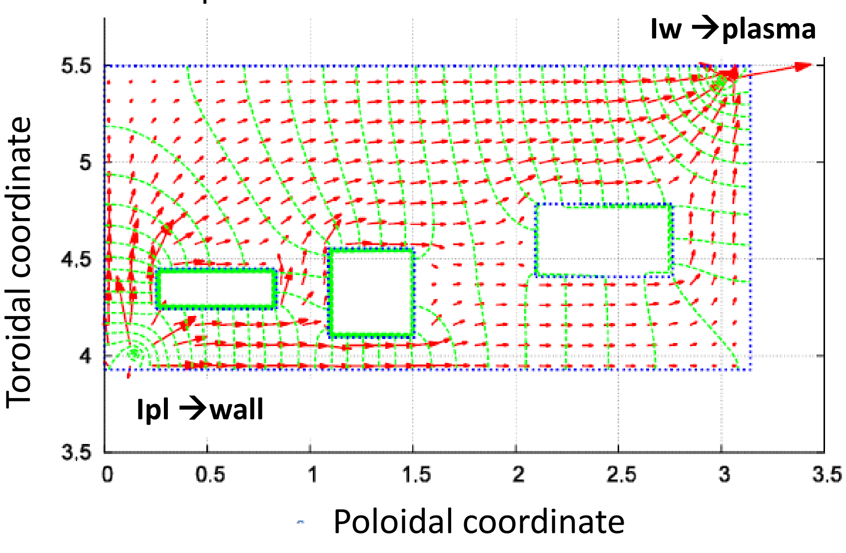
Liaison with international projects: ITER, ITPA

ITER:

- ***ITER has based its Integrated Modelling framework (IMAS) on top of the work done by WPCD: adaptation of EU IM framework and similar data structure (via ITERIS consortium contract)***
- ***Assessment of speed-up techniques to be integrated in SOLPS-ITER***
- ***Develop full 3D codes to describe halo current formation and asymmetries (HLST support):*** extension of STARWALL code with halo currents and its coupling to the non-linear MHD code JOREK

C. Atanasiu

Source potential (green) that allows part of the plasma current to flow into the wall



ITPA benchmarks:

- ***IOS particle transport ITER baseline benchmark***

ETS runs for the whole ITER scenario: ramp up → burning plasma at flat-top → ramp down

- ***Energetic Particles group:***

- benchmark HYMAGYC code for fast ion - MHD interaction

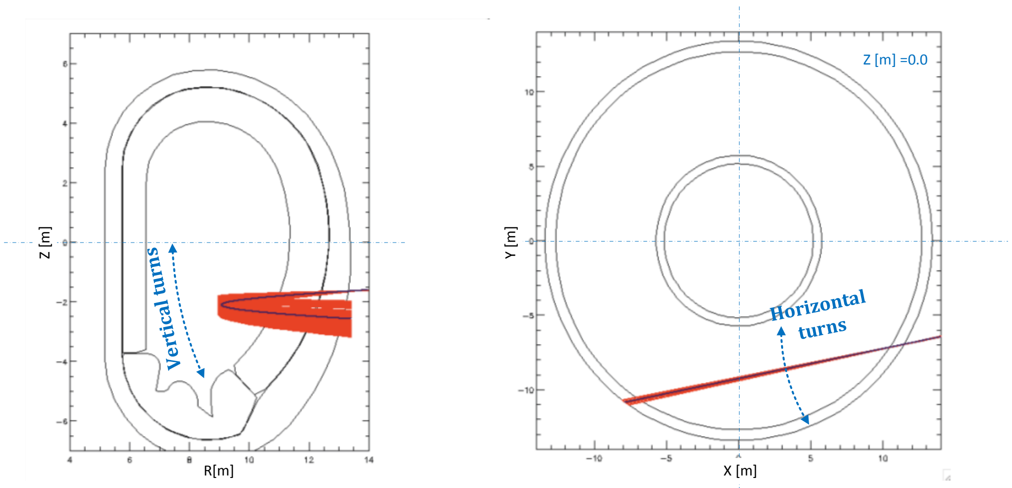
- benchmark of NBI codes using HCD WF

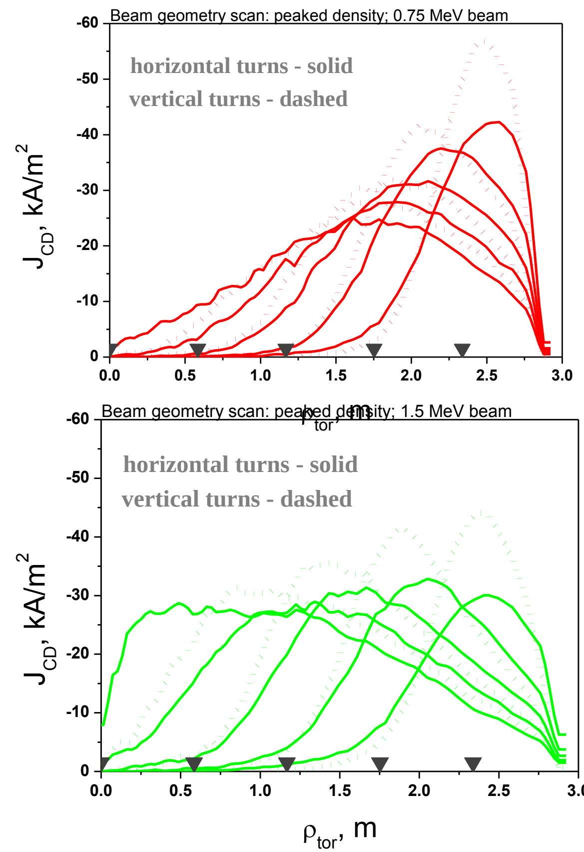
Contribution to DEMO modelling

DEMO:

- ***Pellet modelling and fuelling optimisation, MHD analysis [D. Kalupin et al, EPS 2015]***
- ***NBI simulations: current drive efficiency with different beam configurations and beam neutral energies (ETS, CHEASE, BBNBI, ASCOT) [O. Asunta et al, EPS 2015]***

Denis Kalupin, Rui Coelho, Otto Asunta





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TRANSP applications within EU work programme

- ***TRANSP is actively used within EUROfusion:***

  - analysis/modelling for JET, AUG, MAST-U (talks by H.-T. Kim. G. Tardini, D. Keeling)
  - benchmarking with other EU codes

- ***Application of TRANSP along with other EU codes for analysis and modelling of EU experiments:***

  - Data consistency and diagnostic simulations (including neutron simulations for coming DT campaign at JET)
  - Current diffusion
  - Heating and current drive (NUBEAM, TORIC), fast ion physics
  - Interpretative transport analysis
  - Predictive transport modelling (heat and main particle species, momentum transport)
  - Impurity (non-coronal) simulations
  - Core-edge integration, SOL modelling, plasma-wall interaction
  - Pellet modelling
  - MHD analysis (NTM, sawteeth triggers)

Code color: TRANSP-unique capabilities, common capabilities with other EU codes, presently not available in TRANSP

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