Status Report for WPAC

3rd Theory Project Board | March 10, 2022

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1 – WP Organization

WP AC: Advanced Computing

ACH: Advanced Computing Hubs
- 01: High Performance Computing
  - CIEMAT
  - EPFL
  - MPG
- 02: Integrated Modelling and Control
  - IPPLM
- 03: Data management
  - VTT

HPC: High Performance Computer
- TBD

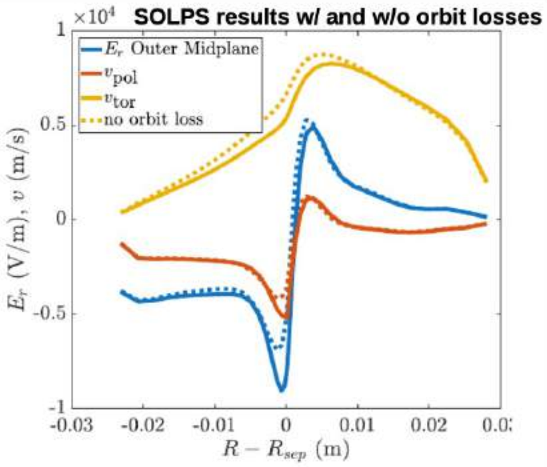
JDC: JET Data Center
- UKAEA

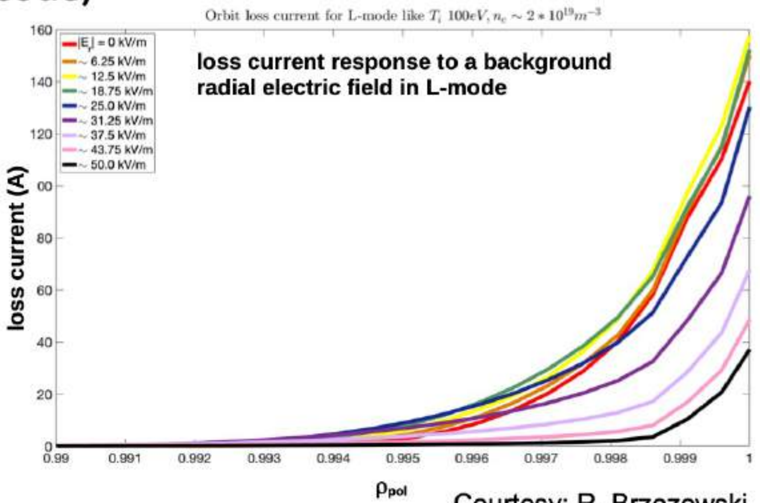
Jet Data Centre hosted by **UKAEA** started to provide services to EUROfusion users (TD-RK-22-19)

TSVV: Theory, Simulation, Validation and Verification
- 01: Physics of the L-H Transition and Pedestals
  - MPG
- 02: Physics Properties of Strongly Shaped Configurations
  - EPFL
- 03: Plasma Particle/Heat Exhaust: Fluid/Gyrofluid Edge Codes
  - CEA
- 04: Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes
  - MPG
- 05: Neutral Gas Dynamics in the Edge
  - FZJ
- 06: Impurity Sources, Transport, and Screening
  - CEA
- 07: Plasma-Wall Interaction in DEMO
  - FZJ
- 08: Integrated Modelling of MHD Events
  - MPG
- 09: Dynamics of Runaway Electrons in Tokamak Disruptions and Start-Up
  - CEA
- 10: Physics of Burning Plasmas
  - MPG
- 11: Validated Frameworks for the Reliable Prediction of Plasma Performance and Operational Limits in Tokamaks
  - MPG
- 12: Stellarator Optimization
  - MPG
- 13: Stellarator Turbulence Simulation
  - CIEMAT
- 14: Multi-Fidelity Systems Code for DEMO
  - UKAEA

D2.1: Ion-orbit loss model

- **Preparing manuscripts for submission: steady-state ion-orbit loss & SOLPS coupling**
  - E_r affected by ion-orbit losses
  - Poloidal asymmetries are less strongly forced
- **Stand-alone orbit loss model with emphasis on clear documentation**
  - largely implemented in GRILLIX (fluid code) with A. Stegmeir; first sims performed
  - shall be ready for TSVV1 (and other) codes hereafter
- **Model accuracy greatly improved** velocity-space coordinates corresponding to losses evolve over a loss trajectory





Courtesy: R. Brzozowski

T. Görler et al. (TSVV1) | 5th E-TASC SB Meeting | Mar 02, 2022 | Page 7

General topic:

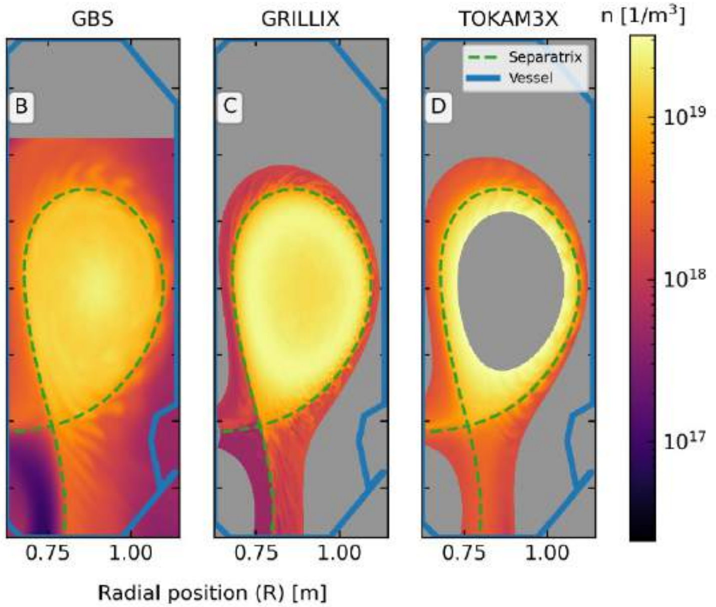
Physics of the L-H transition and pedestals

Key scientific question:

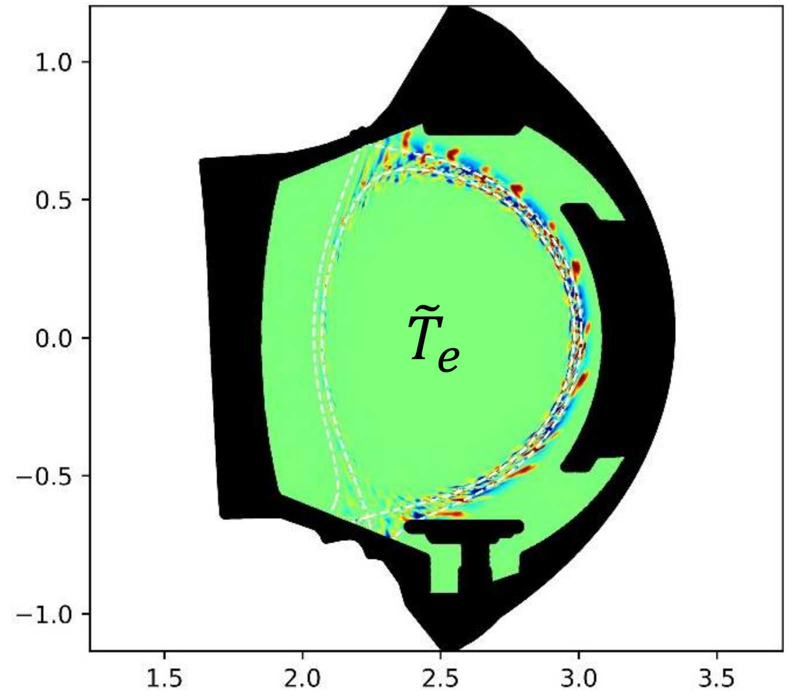
Electric field generation in the edge?

2 – WP Selected Results from 2021: TSVV 03

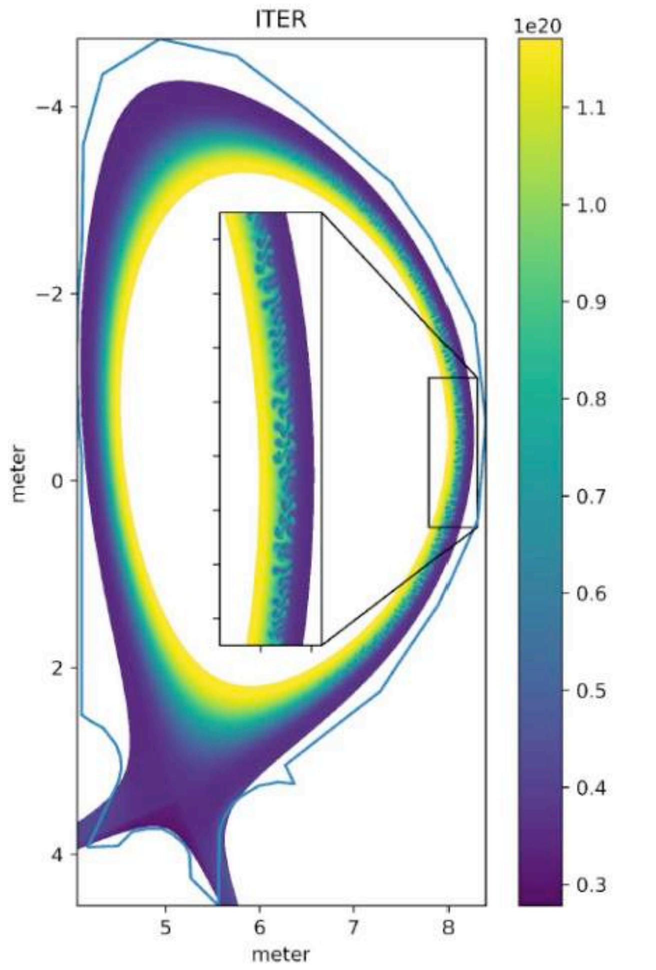
- ❖ Steady progress **towards ITER scale simulations**
- ❖ Latest advances unlock full scale simulations for low $\rho_\star$ machines ($1/\rho_\star \gtrsim 1500$)



GBS/GRILLIX/TOKAM3X TCV simulation (2020)
[Oliveira, Body et al., NF 2022]



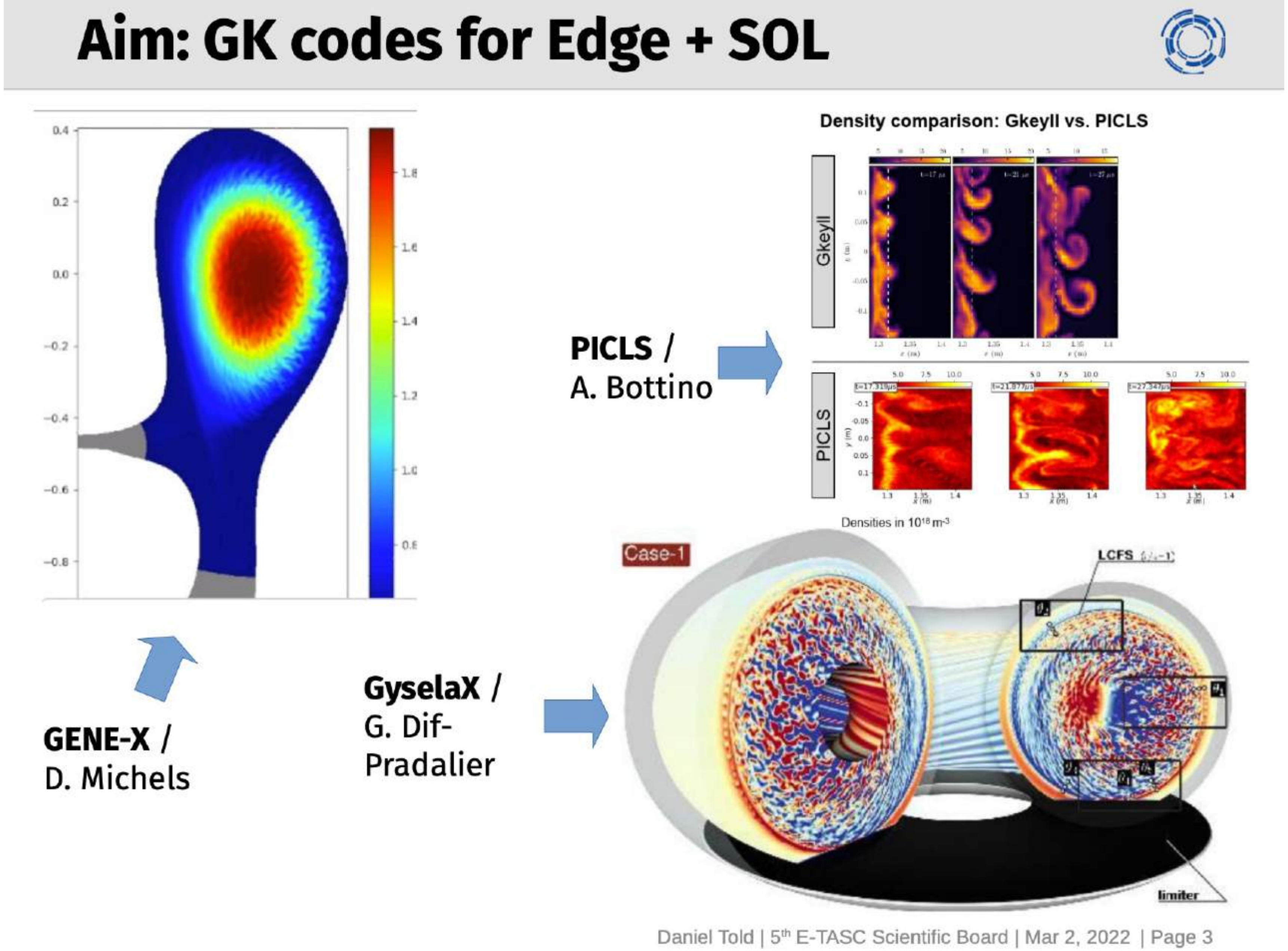
SOLEDGE3X WEST simulations at realistic parameters (1e6 x 128 mesh, 64 nodes)



GRILLIX ITER simulation at realistic parameters (11e6 x 16 mesh, 16 nodes)

Ambitious aim:

Creation of a new generation of gyrokinetic edge turbulence codes



Topic: Neutral gas dynamics in the edge (further development of the EIRENE code)

Requires communication with other TSVVs

Requires ACH support

Physics

- ***Fluid-kinetic hybridisation (FKH)*** *development successfully continues*
- ***A&M CRM*** *improvement (somewhat preparatory work so far…)*
- ***Kinetic ions*** *on the EIRENE side (discussion with TSVV-6)*
- *Establishing* ***simulation cases*** *(validation, ITER, DEMO) – in progress*

Code development

- ***Parallelisation:*** *OpenMP-MPI hybrid (related code refactoring done; optimisation and restructuring e.g. domain decomposition are necessary)*
- ***Code streamlining*** *(Segregation of the numeric core, etc.) – code camp*
- *Improved I/O (JSON/HDF5), visualisation, IMASification, etc. – in progress.*

Organisational items

- ***Repository for simulations*** *(EUDAT?.., using JAC catalogue experience) – concept under development, depends on selection of base system.*
- ***New EIRENE license****, "infectious open source" (draft discussed with FZJ layers and ITER still in circulation)*

KEY DELIVERABLE 2 MILESTONES, DELIVERABLES

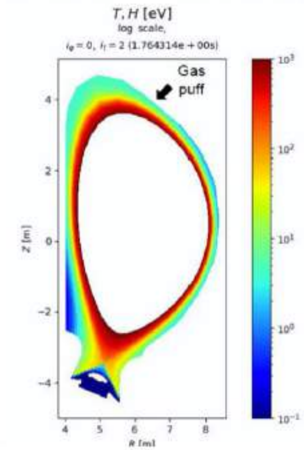
EUROfusion

Key Deliverable 2: Assessment of the W influx, W screening, and W transport in ITER plasmas

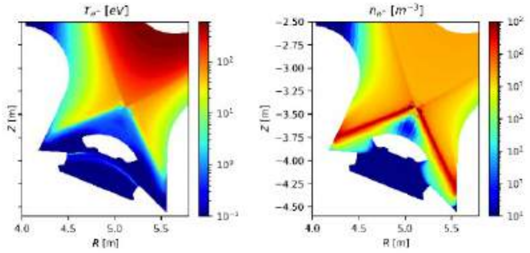
ID	Milestone-description	participants	Target date
M2.1	Review and document ITER scenarios to be modelled	All (site activity managers are responsible for local coordination)	06/2021
M2.2	**2D Plasma background in semi-detached conditions** (no RMP) (both with EMC3-EIRENE and SOLEDGE3X)	**D. Harting**, H. Bufferand, G. Ciraolo, **N. Rivals**	12/2021

Example of ITER simulations with SOLEDGE in 2D

Illustration of case 2297
(mid-upper part of the gas puff scan)



Temperature and density in the divertor region



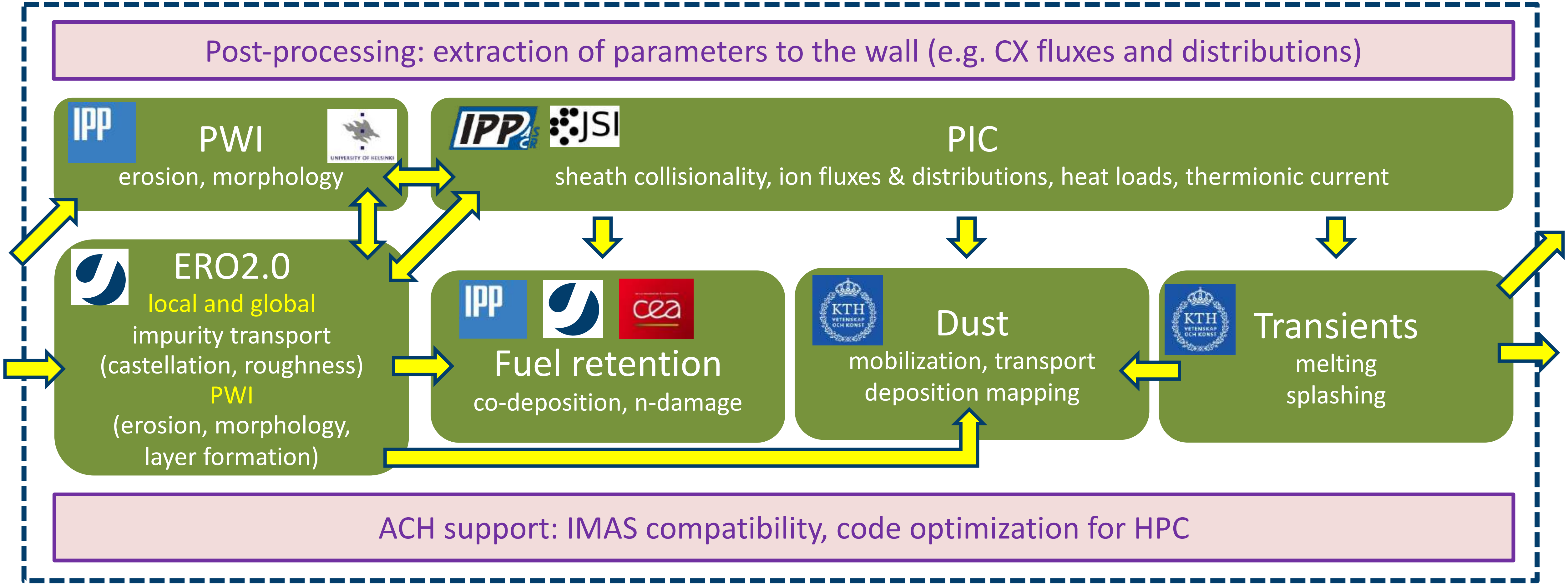
- **Milestone fully achieved**

- *Important progress also on the* ***validation step with ERO2.0*** *applied on impurity transport on W7-X experiments (see for ex. Brezinsek et al Nucl. Fusion 62 016006)*

PWI in DEMO

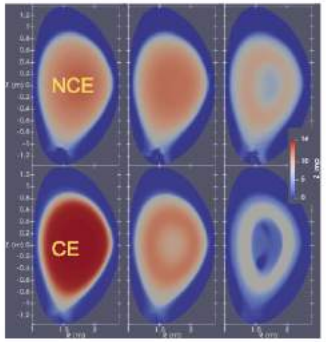
Plasma background, wall geometry, material choice, steady-state and transient heat loads – interaction with WP PWIE, WP DES, DCT, …

Interaction scheme



Working group Disruptions

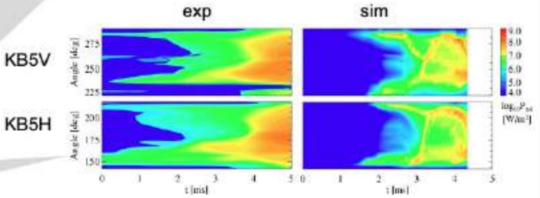
- **Impurity models** were developed for SPI
  - Model *without* coronal equilibrium assumption tracks charge states using pseudo particles (lead by collaborator Di Hu, but with substantial contrib. from TSVV 8 & 9)
  - A simpler model *with* coronal equilibrium assumption
  - Model with kinetic impurities is in development in addition
- **Deuterium, Neon, and mixed SPI** simulations are progressing for JET and ASDEX Upgrade.
  - Validation via direct experiment comparison with virtual diagnostics
- **Benign RE beam termination** studied as observed in JET after secondary D-SPI + extensions for partly ionized impurities (lead by our collaborator Vinodh Bandaru, but with substantial contributions from TSVV 8)
- **Predictive 3D disruption simulations in ITER** done at realistic Lundquist number (of post-TQ plasma) giving insights for dynamics and wall forces; **unmitigated cases** on the way
  - RE transport studied with RE test particles in collaboration with TSVV 9, e.g., trapped particle loss mechanisms
- **Hot VDE simulations** for AUG ongoing including comparison of plasma motion, 3D dynamics, halo currents, etc.
- **Physics of current profile relaxation and Ip spike** investigated



Hu D, Huijsmans GTA, Nardon E, Hoelzl M., et al. PPCF 63, 125003 (2021)

Hu D., Nardon E., Hoelzl M. et al. NF 61, 026015 (2021).

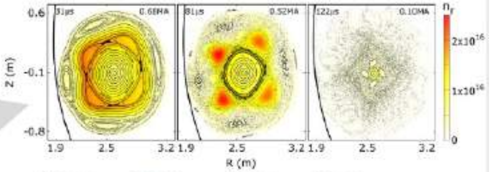
Strien K et al, in preparation



Kong M et al, EFTC 2021, EPS 2022

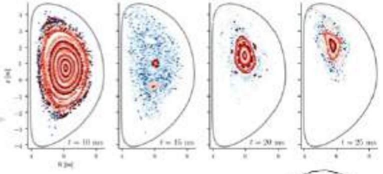
Bonfiglio D et al, EPS 2022

Wieschollek F., Hoelzl M., Nardon E., et al. PoP (accepted)



Reux C., Paz-Soldan C., Aleynikov P., Bandaru V., et al. PRL 126, 175001 (2021)

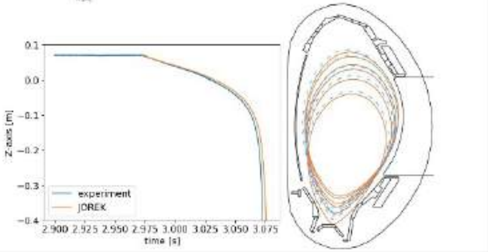
Bandaru V., Hoelzl M., Reux C., et al. PPCF 63, 035024 (2021)



Artola F.J., Loarte A., Hoelzl M., et al. NF (accepted)

Artola FJ, EPS 2022

Särkimäki K., Artola FJ, Hoelzl M, NF (submitted)



Schwarz N et al, EPS 2022 invited

Nardon E., Hu D., Artola FJ, et al. PPCF 63, 115006 (2021)

Sadouni S. et al, in preparation

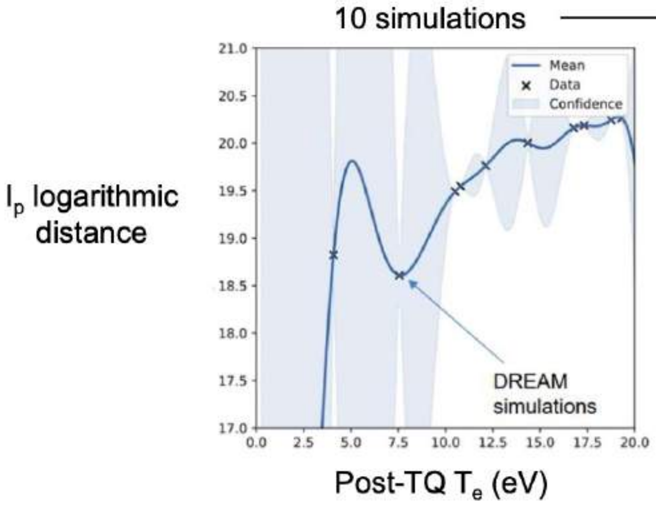
Modelling RE generation with DREAM (1/2)

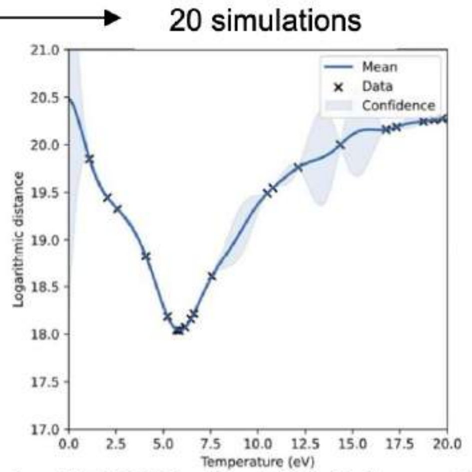
- The **DREAM disruption-oriented kinetic code** [Hoppe CPC 2021]
  - Solves 1D flux surface averaged transport equations (including impurities and effects important in disruptions)
  - Self-consistently evolves the electrons, taking REs into account
    - Various levels of description, from fluid to fully kinetic (2P, bounce-averaged)
  - First application: hot tail RE generation in ITER taking transport in stochastic **B** field into account [Sveningsson PRL 2021]
  - Now **being optimized** with ACH-VTT (implem. of iterative linear solver) and **integrated into IMAS** with ACH-IPPLM

- Work is ongoing towards the **validation** of DREAM regarding RE generation:
  - Simulations of RE formation in JET pulse 95135 [Brandström_MSc_2021]
    - Measurements (e.g. $I_p(t)$) can be ~ matched by tuning input parameters (e.g. post-TQ T_e) → Validation or fancy fit?

→ A **Bayesian framework** has been developed to address this question

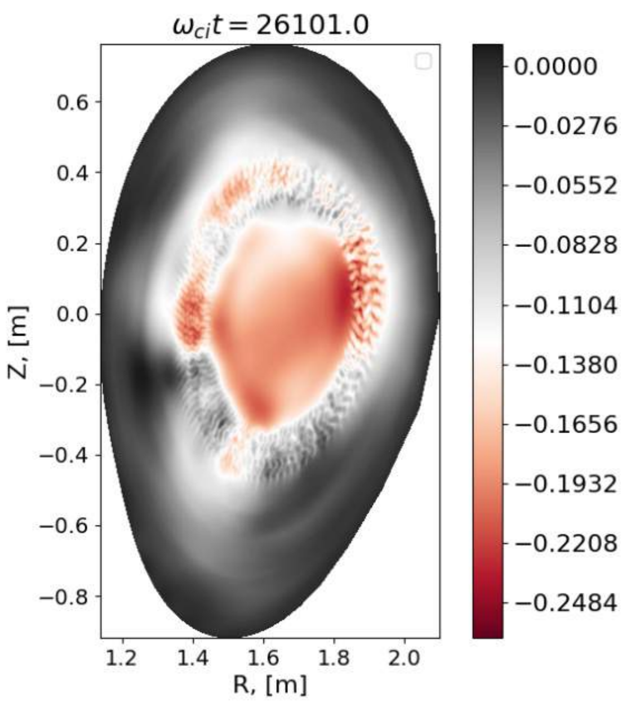
Example: Find post-TQ T_e that minimizes distance between measured and predicted I_p during CQ

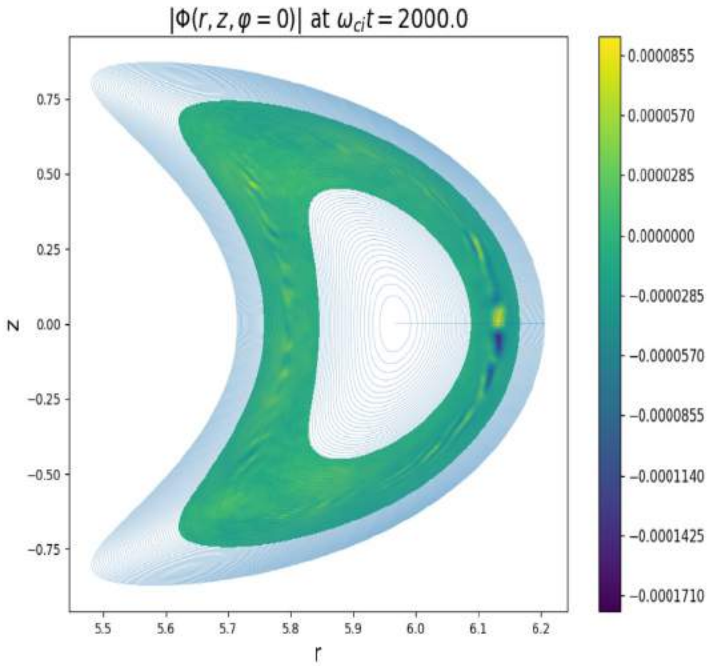


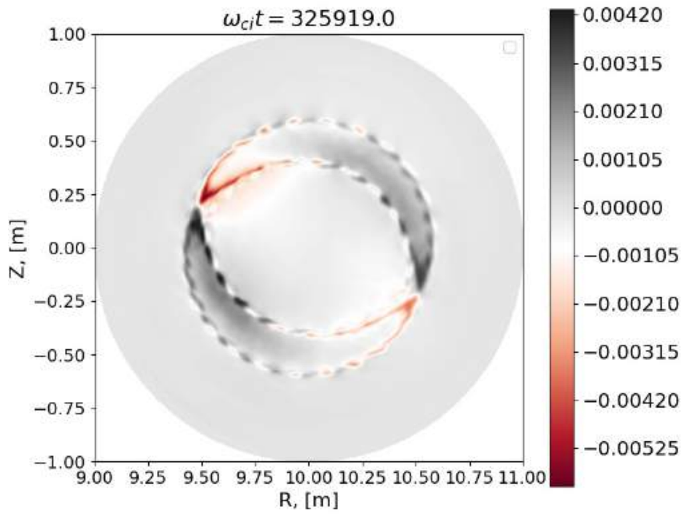


[Järvinen TSVV 9 meeting]

E. Nardon | EUROfusion FSD Science Coord. Meet. | 18 Jan. 2022 | Page 3







Extensions to other physics (meso-/micro-scale couplings):
(1) Tearing instability: interaction with EM turbulence
(2) Alfvenic (e.g., TAEs) + fast ions + EM turbulence (ITGs) + ZF

Global electromagnetic turbulence in ASDEX Upgrade and W7-X

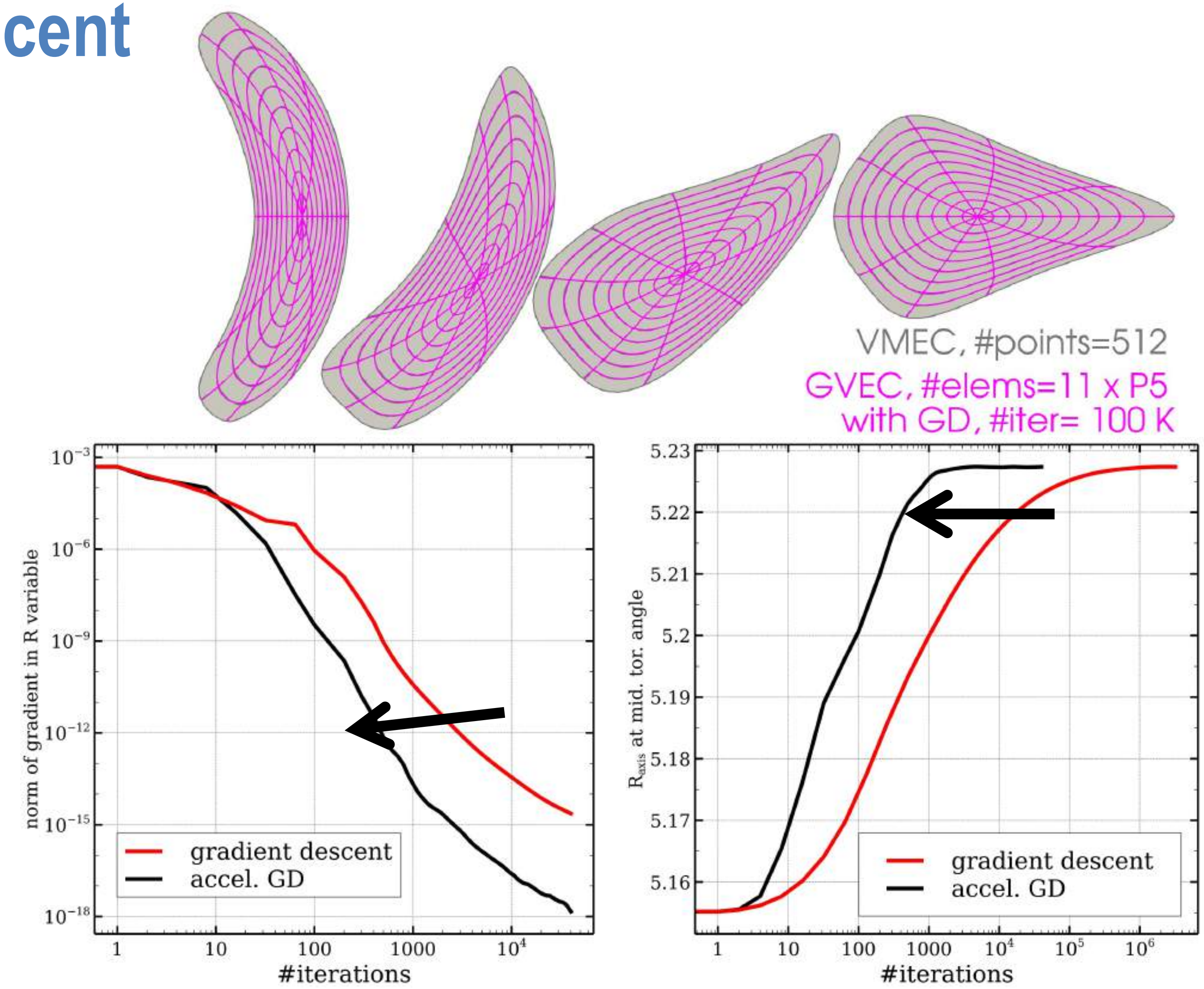
(1) Numerically accessible on existing HPC systems

(2) Detailed physics studies and algorithmic improvements ongoing

(3) Extensions to other machines (e.g., JET & TCV) are desirable

GVEC – Accelerated Gradient Descent

- Tested on W7-X fixed boundary case (compared to VMEC)
- When iterating to very small force residuals, undesired solution features appear (not clear why, possibly related to missing angular constraint)
- Accelerated gradient descent needs **factor 10-100 less iterations** to converge (forces, axis position) compared to gradient descent



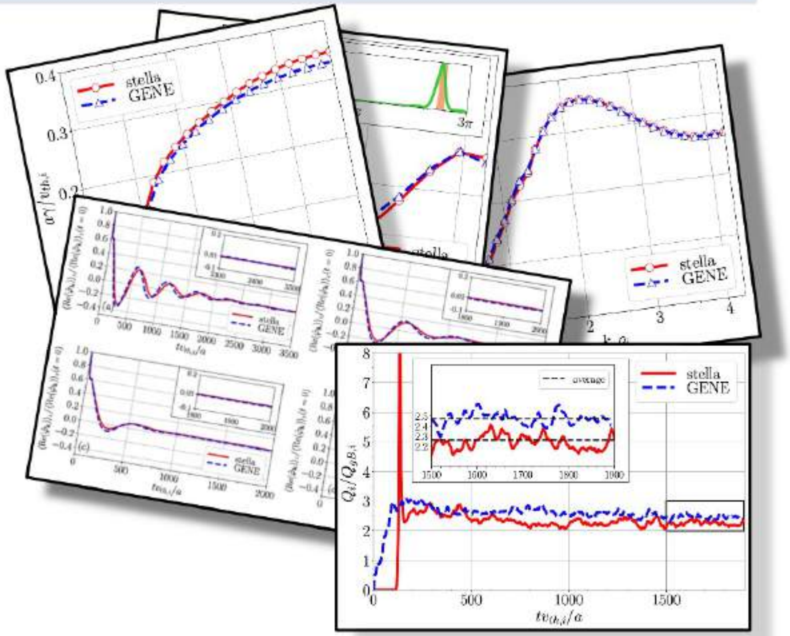
Deliverables in 2021

Deliverable ID / Short name	Key deliverable(s)	Due date
D1.1 / D-REF-CASES	1, 3, 4	March 2021
Agreed W7-X reference case and set of **representative OP2 operation scenarios** for **comparisons, benchmark activities.**		
D1.2 / D-TURB-ZTRANSP	3, 4	~~Dec. 2021~~ → 2022
Study of the **effect of collisions on the background turbulence and impurity transport** in multispecies electrostatic flux tube simulations.		

Turbulent transport in stellarators

	Flux tube	$[N_\theta^m, N_\theta^M]$	a/L_{T_i}	a/L_{n_i}	N_z	$N_{v_\parallel}$	N_μ	$N_{\mathbf{k},j}$	$\Delta t v_{\mathrm{th},i}/a$	Compared
Test 1.	bean	[1 , 6]	3	1	256	36	24	Off	stella 0.15 GENE 0.14	$\gamma(k_x)$, $\omega(k_x)$ $\gamma(k_y)$, $\omega(k_y)$
Test 2.	triangular	[4 , 6]	3	1	512	36	24	Off	stella 0.15 GENE 0.14	$\gamma(k_x)$, $\omega(k_x)$
Test 3.	bean	[2 , 8]	0	3	512	36	24	Off	stella 0.04 GENE 0.004	$\gamma(k_y)$, $\omega(k_y)$ $\lvert\hat{\varphi}_{\mathbf{k}}\rvert(z)$
Test 4.	bean	[4 , 4]	0	0	512	256	32	Off	stella 0.15 GENE 0.1	$\langle \mathrm{Re}(\hat{\varphi}_{\mathbf{k}}) \rangle_z(t)$
Test 5.	bean††	[1 , 1]	3	1	128	60	24	On	stella 0.09 GENE 0.09	$Q_i(t)$ $\sum_{k_y} Q_i(k_x, k_y)$ $\sum_{k_x} Q_i(k_x, k_y)$

[González-Jerez submitted'21]



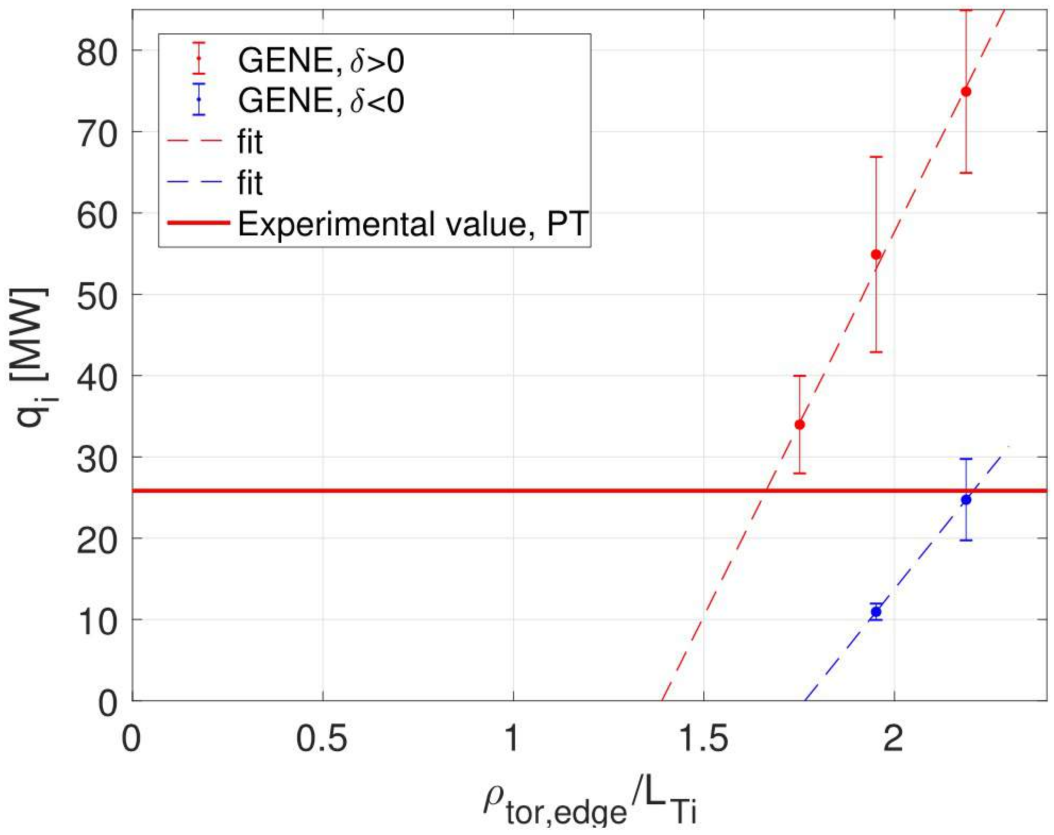
Scientific highlights - Verifying reduced models

A. Mariani, A. Balestri, I. Casiraghi, P. Mantica.

Scientific issue:

What are the prospects of NT plasmas?

- High-fidelity, realistic local GENE simulations of ITG-dominated iDTT scenario
- NT reduces the heat flux by >50%, corresponding to a 10-30% increase in R/L_{Ti}
- Plan to benchmark such GENE studies against TGLF integrated modeling



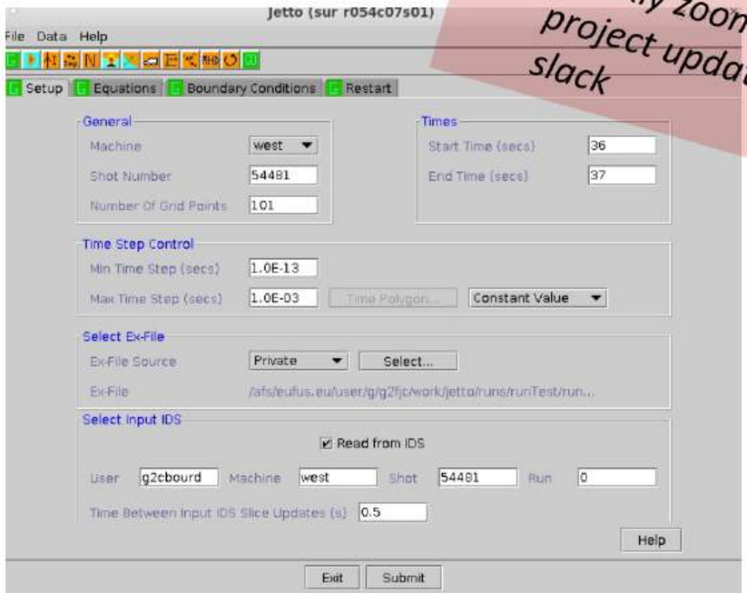
2 – WP Selected Results from 2021: TSVV 11

WP1: HFPSeu Workflow orchestration and module coupling framework

- What is the High Fidelity Pulse Simulator?
  - Python workflow based on **IMASified JINTRAC (i.e. JETTO+EDGE2D)** developed within a CCFE-ITER contract, workhorse for scenario preparation in ITER Physics Dept.
  - Building on ITM/WPCD/CPT/ITER previous work: **any IMASified physics module can be included in the python workflow**, already the case for the WPCD developed Heating and Current Drive module. NB: even the core transport solver could be replaced if physics driven needs exist.

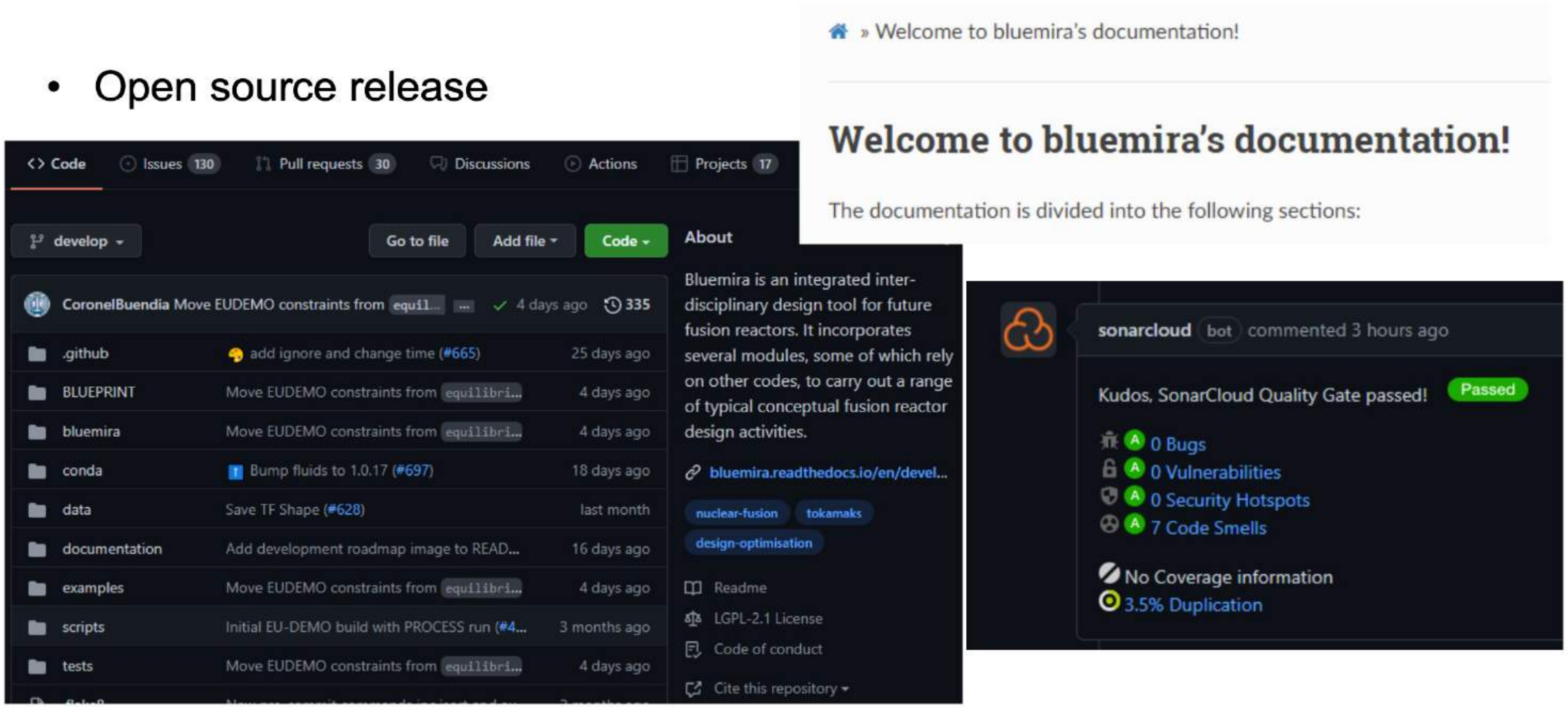
- Present status:
  - **HFPS components have been compiled and installed natively on the EuroFusion Gateway**. 2 training took place, and all documentation available from TSVV11 wikipages.
  - Detailed plans for containerised IMAS workflows in place with ACH Poznan.
  - HFPS GUI: plan in place for short term improvements to aid usability with ACH Poznan
  - DevOps: Now being put in place thanks to EUROfusion package awarded to ACH Poznan
  - Coupled to experimental IDS from AUG, JET, TCV, WEST see wiki.

Very good synergy with ACH Poznan, weekly zoom for project update, Trello, slack



Main Achievements

- Open source release



D. Short | TSVV-14 E-TASC Update | 02.Mar.2022 | Page 4

2 – Progress Towards EUROfusion Standard Software

Progress towards EUROfusion Standard Software

	SOFTWARE ENGINEERING				INTERFACES			VVUQ				DISSEMINATION		DOCUMENTATION		USER SUPPORT	
ACH support start in 2 2022	1. Version control implemented	2. Software engineering rds	3. Coding standards established	4. Performance optimization on HPC s	1. User-friendly interface	2. Post-processing and visualisation	3. Interface to the IMAS Data ary	1. Specific plans for code verification	2. Code verification studies plished	3. Inter-code benchmarking plished	4. Code validation studies plished	1. Up-to-date release version on teway	2. Trainings provided to code	1. High-quality technical entation	2. User manual available for ad	1. Responsive support team	2. Tools for managing support ts
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Not started	Completed	Completed	Completed	Not started	N.A.	Completed	In Progress	N.A.	Completed	Not started	In Progress	In Progress	N.A.	Completed	In Progress	Completed	Completed
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In Progress	Completed	Completed	In Progress	In Progress	N.A.	Completed	N.A.	In Progress	Not started	In Progress	Completed	Not started	Not started	Not started	Not started	In Progress	Not started
In Progress	Completed	Completed	In Progress	In Progress	N.A.	In Progress	Not started	In Progress	In Progress	In Progress	Not started	Not started	Not started	In Progress	In Progress	In Progress	Not started
In Progress	In Progress	In Progress	Not started	Not started	Not started	In Progress	Not started	Completed	In Progress	Not started	In Progress	Not started	Not started	In Progress	In Progress	Completed	Not started
In Progress	Not started	Completed	Completed	Not started	N.A.	N.A.	Completed	Completed	Completed	Not started	Completed	Not started	Not started	Not started	Not started	Not started	Not started
In Progress	Completed	In Progress	In Progress	Not started	Not started	Completed	Not started	Not started	Completed	Not started	In Progress	Not started	Not started	In Progress	In Progress	Completed	Completed
In Progress	Completed	In Progress	In Progress	Not started	In Progress	In Progress	Not started	In Progress	Completed	Not started	In Progress	Not started	Not started	Completed	In Progress	In Progress	Not started
In Progress	Completed	Completed	In Progress	In Progress	N.A.	Completed	Not started	In Progress	In Progress	Not started	N.A.	Not started	Not started	In Progress	In Progress	In Progress	Completed

Good progress in many areas

More work needed:

- Performance optimization
- IMAS interfaces
- Inter-code benchmarking
- Dissemination
- User support

2 – Available ACH Support

Total ACH resources: baseline = overall available resources minus 10% (1680 PM = 140 PY)

Distribution of the total ACH resources over the 14 TSVVs:

TSVV-1: 10/113 ~ 12.4 PY

TSVV-2: 5/113 ~ 6.2 PY

TSVV-3: 10/113 ~ 12.4 PY

TSVV-4: 10/113 ~ 12.4 PY

TSVV-5: 7/113 ~ 8.7 PY

TSVV-6: 5/113 ~ 6.2 PY

TSVV-7: 10/113 ~ 12.4 PY

TSVV-8: 10/113 ~ 12.4 PY

TSVV-9: 6/113 ~ 7.4 PY

TSVV-10: 10/113 ~ 12.4 PY

TSVV-11: 10/113 ~ 12.4 PY

TSVV-12: 10/113 ~ 12.4 PY

TSVV-13: 7/113 ~ 8.7 PY

TSVV-14: 3/113 ~ 3.7 PY

Nominal usage profile: Suggested usage of ACH resources by the end of...

2021: 6.5%

2022: 24.8%

2023: 47.4%

2024: 73.6%

2025: 100%

3 – Status of Grant Milestones & Grant Deliverables (2021)

GA Deliverable No.	Title	Due Date	Status	Details on Status (in case of delays or issues)
D04.01	Establishment of six Advanced Computing Hubs including JET data centre	31/12/2021	Completed	
D04.02	KPI for 2021 on high availability of HPC and Gateway resources in support of physics and engineering programme reached	31/12/2021	Cancelled	To be cancelled due to duplication between FP8 and FP9 Grant Deliverables. The activity is funded from FP8, therefore deliverables shall not appear in FP9.

GA Milestone No.	Title	Due Date	Status	Details on Status (in case of delays or issues)
M04.01	TSVV kick-off meeting performed. Interfaces for collaboration between TSVVs and WPs defined and established	31/12/2021	Completed	
M04.02	Decision on the location of the Advanced Computing Hubs and resources	31/12/2021	Completed	
M04.03	Availability (defined by KPIs) of Gateway and HPC to EUROfusion users for production runs	31/12/2021	Completed	
M04.04	Decision on the new HPC and Gateway for the EUROfusion programme beyond 2023	31/12/2021	Delayed	The technical requirements are defined, however the available budget is still unclear.

4 – Risk & Mitigation Register: Current Status

Description of Risk	Severity	Likely hood	Proposed Mitigation Action	Risk materialized?	Mitigating Measures applied?	Comments
Not all Advanced Computational Hubs up and running	M	L	Resource levelling and reprioritization	no	n.a.	All hubs are running; the work is very much appreciated by code owners (TSVVs)
Available resources not sufficient for provision of the set of codes	M	M	Reprioritization and down selection of the codes	no	n.a.	From 2022, TSVVs are running at the full speed; ACHs will reach their full capacity in 2023
Reduced HPC availability for scientific use	M	M	Resource levelling and reprioritization	no	n.a.	So far, HPC operation is stable and guaranteed until the end of 2023
Absence of IMASified data from EUROfusion experiments for code validation	M	L	Resource levelling and reprioritization; act at a broader EUROfusion level to make such data available (action A5); collaboration on V&V activities with ITER IO	no	n.a.	For the current development stage, this risk is not important; it might become critical towards the end of the programme in 2024-2025, when codes are supposed to demonstrate their full capabilities

Decisions on PCRs

PCR Number	PCR Title	PCR Status	Comments
CR1	Approval of change request to ACH-VTT programme 2022	approved	The PB approved the CR1. (https://indico.euro-fusion.org/event/1192/)
CR2	Minor changes to PMP (E.Sanches/CIEMAT)	implemented	The PB took note on CR2 (as it is a minor editorial change to the PMP). FSD CO updated the document accordingly. (https://indico.euro-fusion.org/event/1192/)
CR3	Corrections to ACH-CIEMAT tasks to be carried in 2022	requested	The assessment of support tasks requested for BLUEMIRA code (TSVV-14) have indicated the mismatch between the task nature and the ACH profile. Correction measures: • Re-distribute 12 PMs originally foreseen for the task to support of other codes managed by ACH-CIEMAT; • Provide support to BLUEMIRA code in 2023 through other ACH. *The request has been recommended by the E-TASC SB at its meeting on March 3, 2022*

6 – AOB: Some General Points

About one year into E-TASC, it is noticable that we are picking up momentum

TSVVs are gaining ground in key scientific areas

ACHs are already providing significant support, with more to come

Project can be thought of as a "team of teams"

All TSVVs call for a serious mission budget

Will be working on a NJP Roadmap paper

More details and original documents (recent E-TASC SB meeting) can be found here:

https://indico.euro-fusion.org/event/1824
https://indico.euro-fusion.org/event/1825