Status Report for the DSD WP AC

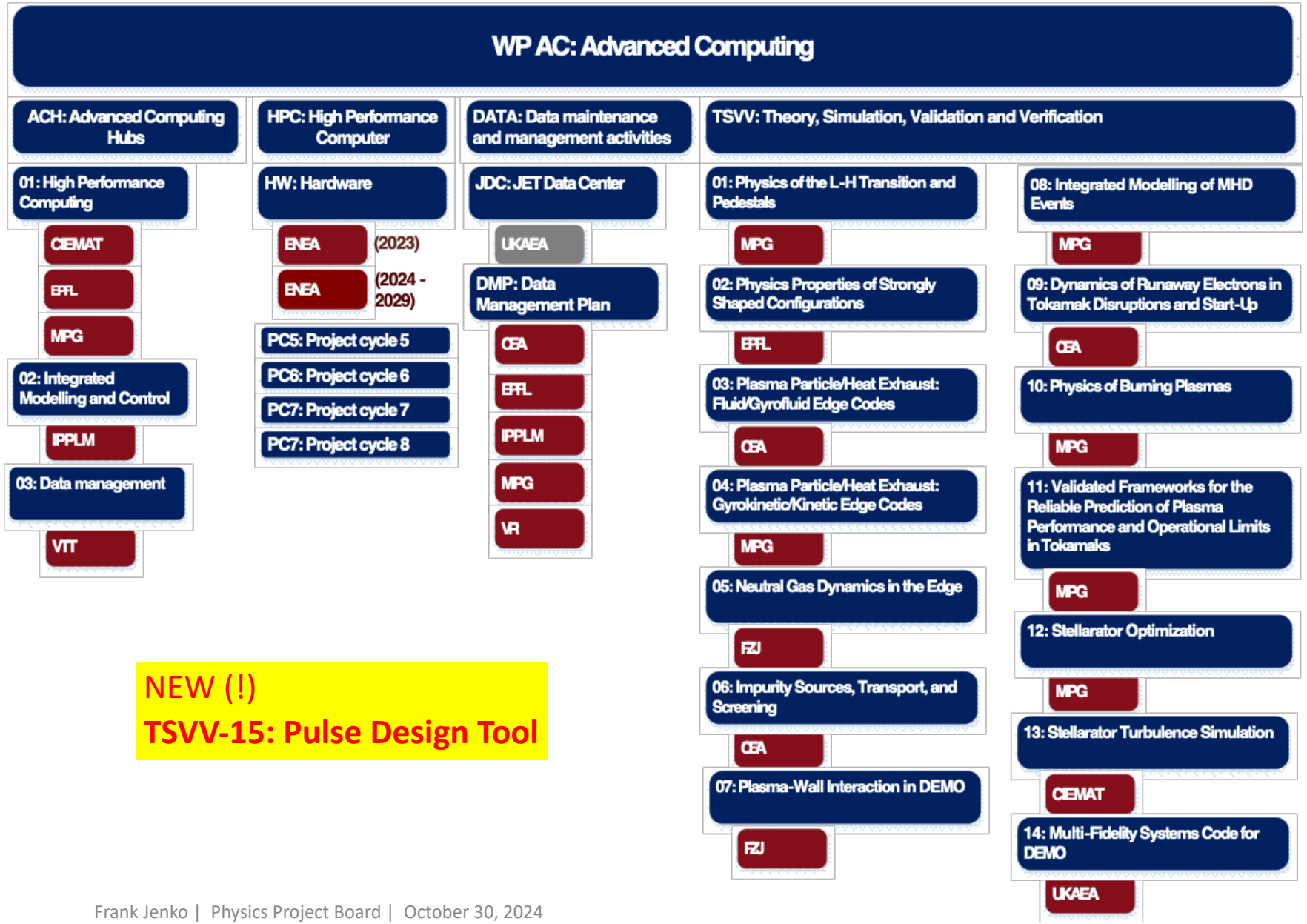
Physics Project Board | October 30, 2024

F. Jenko (with D. Kalupin and V. Naulin)

Thanks to contributions by the E-TASC SB

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Organization of WP AC



NEW (!)
TSVV-15: Pulse Design Tool

WP AC objectives are to run a coherent program of TSVV projects and to develop a suite of "EUROfusion Standard" software

Scientific objectives TSVVs were pre-defined by the E-TASC SB, prior to the TSVV CfP (2021-2025)

Scientific objectives ACHs are defined following requests by code developers with approval by the E-TASC SB (annually)

Monitoring of activities is by the E-TASC SB and the PMU

TSVV selection & monitoring (by E-TASC SB)

EUROfusion

Call: Spring 2020

TSVV Task 1: Physics of the L-H Transition and Pedestals

Expected resources: Up to about 10 ppy per year (incl. about 30% for ACH personnel)

Background

Regarding the plasma core, present-day gyrokinetic (GK) simulations of turbulent transport may be characterized as relatively mature, allowing for quantitative comparisons with measurements on a regular basis. Meanwhile, an important new frontier of GK is to advance towards a comprehensive, self-consistent description of the pedestal/edge region, including the physics of the L-H transition. The time is ripe to address these outstanding challenges, building on years of preliminary work and exploiting the capabilities of emerging exascale supercomputers.

Initial applications of GK codes to the near-edge region of tokamak plasmas over the last decade or so have highlighted the importance of a range of physical effects, calling for global simulations in realistic magnetic geometries – involving electromagnetic effects, high-quality collision operators, and the ability to retain both sub-ion-scale fluctuations and relevant macroscopic (MHD-like) instabilities. Moreover, GK codes have demonstrated the capability to reproduce experimentally measured fluxes in near-edge L-mode plasmas and have been used to explore to some degree the residual turbulent transport in H-, QH-, and I-mode pedestals. In addition, full-f GK codes applicable to the edge and SOL are being developed (see TSVV Task 4), providing new ways to attack the L-H transition problem. Another key aspect of the present TSVV task is the development of validated and fast reduced transport models – on the basis of the GK simulations – to be used in integrated modelling codes.

Aims of the project

- Capability to carry out self-consistent, robust, and validated GK simulations of L-H transitions and to accurately predict the pedestal profiles; extension to QH-/I-mode discharges.
- Validated and fast reduced transport models which can be used for multi-channel core-edge predictive modelling.
- Applications of GK simulations and reduced models to (natural or controlled) small/no ELM regimes, studying their transferability to ITER and DEMO.

Key deliverables

1. Validated local and global (electromagnetic, collisional) GK simulations of ion-scale, electron-scale, and multi-scale turbulent transport in the H-, QH-, I-, and L-mode edge.
2. Extension of these simulations to self-consistently include relevant macroscopic (MHD-like) instabilities and the development of a radial electric field.
3. Consistent application of at least one edge GK code (developed in TSVV Task 4) – which is able to bridge the core, pedestal, and SOL regions and includes neutral physics – to the L-H transition problem.
4. An interpretative and predictive capability of L-H transitions (based on a sound validation strategy and ideally also including extensions to QH-/I-mode discharges) accurately capturing the observed edge plasma dynamics in various machines.
5. Reduced transport models for the pedestal on the basis of GK simulations, involving electron-scale, ion-scale, and macroscopic (MHD-like) instabilities; these can then be included in MHD and transport studies, exploiting synergies with TSVV Tasks 8 and 11.

Detailed workplan with timeline, milestones, SMART deliverables, and risk assessment (2021-25)

Mid-term review of Theory Simulation Verification & Validation (TSVV) projects 2021-2025 by the E-TASC Scientific Board

Mid-term review: Fall 2023

Purpose of the review

The goal of this review is to assess the TSVV projects' performance, the achievements in computational science and plasma physics, the efficiency of the project management, and the project's broader impacts on the EUROfusion programme and the wider scientific community.

The project achievements are considered, along with possible deviations from the original proposal. Specific challenges and opportunities are identified, and changes to project priorities, activities and objectives are proposed.

Furthermore, on a higher level, additional synergetic interactions between projects in EUROfusion and adjustments to the overall project portfolio are proposed.

Methodology

The review was carried out as a three-step process:

- Presentation of each TSVV project's achievements to date to a broad audience of EUROfusion scientists, focusing on the main scientific and technical highlights, briefly mentioning specific impacts (achieved or anticipated) on the WPs, and plans. All materials are available at https://indico.euro-fusion.org/event/2429/

ACH selection & monitoring (by E-TASC SB)

Call: Spring 2020

EUROfusion

EUROfusion · Boltzmannstr. 2 · 85748 Garching · Germany

PROGRAMME MANAGEMENT UNIT
Tony Donné
Programme Manager

Phone: +49 89 3299-4201
Fax: +49 89 3299-4299
tony.donne@euro-fusion.org

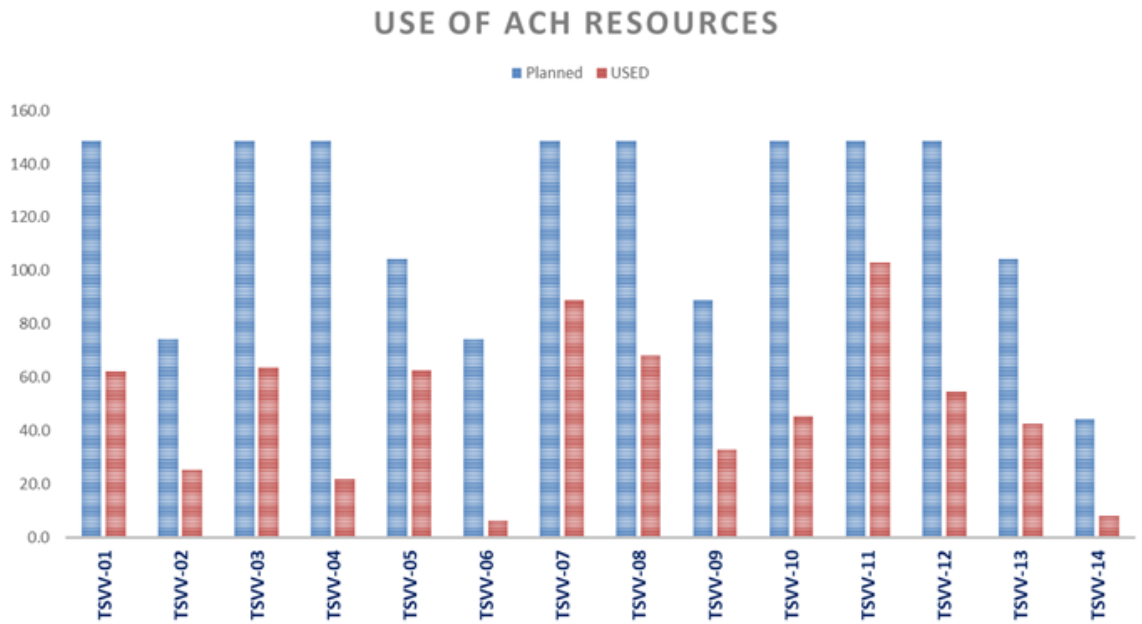
Our ref: PMU/1740

Date: 12th May 2020

To the Members of the General Assembly

Subject: Work Plan for the Implementation of the Fusion Roadmap in 2021 – 2025: Call for proposals for hosting *Advanced Computing Hubs* within the *EUROfusion – Theory and Advanced Simulation Coordination (E-TASC)*

Mid-term review: Spring 2024



	Year	ACH	Customer Project/WP	Code	Project Coordinator	PM's requested	PM's assigned	ACH team members	Tasks description	Comments
11	2021	EPFL	TSVV-10	EUTERPE		2,0	0,5	Lanti	Further development of GPU functionality (OpenACC) for large-scale EM turbulence simulations;	
12	2021	EPFL	TSVV-13	EUTERPE		2,0	0,0	To be hired in eM+	Development and application of tools for advanced visualization of 3D data resulting from global	
13	2021	EPFL	TSVV-03	FELTOR		1,5	0,5			task distributed per code
14	2021	EPFL	TSVV-03	GBS		1,5	0,5			task distributed per code
15	2021	EPFL	TSVV-03	GBS		1,2	1,0	Lanti	Optimization of kinetic neutrals treatment (method of characteristics and coupling to EIRENE)	
16	2021	EPFL	TSVV-03	GBS		6,0	1,0	Peybernes/Varini	Code profiling and optimization	
17	2021	EPFL	TSVV-03	GRILLIX		1,5	0,5			task distributed per code
18	2021	EPFL	TSVV-03	GRILLIX		6,0	1,0	Peybernes/Varini	Code profiling and optimization	
19	2021	EPFL	TSVV-01	GYSELA		1,5	1,0	Peybernes	Support for GPU porting and increased vectorisation for ARM-based architectures	
20	2021	EPFL	TSVV-04	GYSELA		1,5	1,0	Peybernes	Support for GPU porting and increased vectorisation for ARM-based architectures	
21	2021	EPFL	ACH	management	Paolo Ricci	1,5	1,5	Paolo Ricci	management of ACH activities	
22	2021	EPFL	TSVV-01	ORB5		4,0	1,0	Lanti	Improve multi-threading of ORB5 & particularly of its field solver. Adaptations to the M100	
23	2021	EPFL	TSVV-02	ORB5		4,0	1,0	Lanti	Improve multi-threading of ORB5 and particularly of its field solver. Adaptations to the M100	
24	2021	EPFL	TSVV-09	ORB5		4,0	1,0	Lanti	Further development of GPU functionality (OpenACC) for large-scale EM turbulence simulations;	task distributed per code
25	2021	EPFL	TSVV-10	ORB5		2,0	0,5	Lanti	Further development of GPU functionality (OpenACC) for large-scale EM turbulence simulations;	task distributed per code
26	2021	EPFL	TSVV-03	SOLEDGE3X		1,5	0,5	Varini	Poisson solver optimization, including porting to GPU	
27	2021	EPFL	TSVV-06	SOLEDGE3X		3,0	1,0	Peybernes/Varini	Profiling and optimisation of SOLEDGE3X in the case of high number of species	
28	2021	EPFL	TSVV-01	Various codes		2,0	0,0	To be hired in eM+	Development of community visualisation tools that will enable us to easily navigate the huge	
29	2021	IPPLM	ALL	AAI	Liviu Joita	5,0	5,0	Pawel Spychala	AAI Infrastructure Rollout and support	
30	2021	IPPLM	TSVV-12	ASCOT5	Per	0,5	0,2	Michal Poradzinski	ASCOT5. Implementation in IMAS framework	
31	2021	IPPLM	TSVV-12	BEAMS3D	Per	0,5	0,2	Michal Poradzinski	BEAMS3D. Implementation in IMAS framework	
32	2021	IPPLM	TSVV-07	BIT1	Dmitry	2,5	0,2	Dimitriy Yadykin	code adaptation to IMAS, focusing firstly on IMAS compatible outputs.BIT-1D, BIT-3D	
33	2021	IPPLM	TSVV-03	DATABASES	Patrick	6,0	2,5	Daniel Figat	This task is led by VTT ACH. We can help with the Repository and Continuous Integration	
34	2021	IPPLM	TSVV-11	DATABASES	Clarisse	3,0	1,0	Dimitriy Yadykin	Initial implementation of multimachine remote data gathering and (for 1D profiles) fitting using	
35	2021	IPPLM	ALL	DEVOPS	Clarisse	2,4	3,0	Daniel Figat	Aid with setup and maintenance of potential new DevOps platform and documentation. To be	
36	2021	IPPLM	TSVV-09	DREAM	Eric Nardon	6,0	0,5	Dimitriy Yadykin	DREAM.Integration into IMAS	
37	2021	IPPLM	TSVV-11	DYON	Clarisse	1,2	0,0	Michal Owsiak	Adapt DYON to IMAS and containerise (and adapt from matlab to octave or python)	
38	2021	IPPLM	TSVV-05	EIRENE	Dmitriy	0,5	0,2	Dimitriy Yadykin	Integration of code I/O in the IMAS:	
39	2021	IPPLM	TSVV-07	ERO2.0	Dmitry	2,5	0,2	Dimitriy Yadykin	code adaptation to IMAS, focusing firstly on IMAS compatible outputs.ERO2.0	
40	2021	IPPLM	ALL	ETS	Par Strand	3,9	3,9	Par Strand	ACH-workflows/ETS	
41	2021	IPPLM	TSVV-03	FELTOR		1,5	0,1			task distributed per code
42	2021	IPPLM	TSVV-03	GBS		1,5	0,1			task distributed per code
43	2021	IPPLM	TSVV-02	GENE	Justin Ball	0,0	0,2	Michal Poradzinski	Ensure IMAS compatibility of software. All codes (GENE, ORB5, GBS, HYMAGYC, XTOR)	
44	2021	IPPLM	TSVV-03	GRILLIX		1,5	0,1			task distributed per code
45	2021	IPPLM	TSVV-11	HPPS	Clarisse	3,0	3,0	Bartosz Bosak	Containerise HCD workflow (Docker)	
46	2021	IPPLM	TSVV-11	HPPS	Clarisse	1,2	2,0	Piotr Grabowski	Give input into concept design for a generic python GUI - cloud native, web based, data driven	
47	2021	IPPLM	TSVV-11	HPPS	Clarisse	1,8	1,0	Barek Palak	Adapt existing HPPS python components from FC2K to Iwrap	
48	2021	IPPLM	TSVV-11	HPPS	Clarisse	2,4	3,0	Daniel Figat	Setup common IMAS-python workflow testing framework. Add CI build and run tests for HPPS	
49	2021	IPPLM	TSVV-11	HPPS	Clarisse	3,0	2,0	Bartek Palak	Adapt existing Kepler based components to IMAS Python workflows and Iwrap	
50	2021	IPPLM	TSVV-11	HPPS	Clarisse	0,6	0,0	Dimitriy Yadykin	Provide SOL models (as in Luda NF2020 for example) parameterisation as a simple IMAS python	
51	2021	IPPLM	ALL	IMAS	Marcin	8,0	8,0	Marcin Plociennik	IMAS Ecosystem Infrastructure support+maintanance+deployments	
52	2021	IPPLM	TSVV-01	IMAS	Tobias	1,0	0,2	Michal Owsiak	IMAS code output support/training	
53	2021	IPPLM	TSVV-10	IMAS	Oleksiy	2,0	2,0	Par Strand	Up-to-date IMAS support including ITER/WPCD integrated modeling tools, experimental data	
54	2021	IPPLM	TSVV-11	IMAS	Clarisse	1,2	1,0	Tomasz Zok	Design python IMAS workflows for multiple containers, use JINTRAC-HCD as template / proof of	
55	2021	IPPLM	TSVV-11	IMAS	Clarisse	1,2	1,0	Bartosz Bosak	Containerise NICE (Docker)	

ACH mid-term review: Recommendations

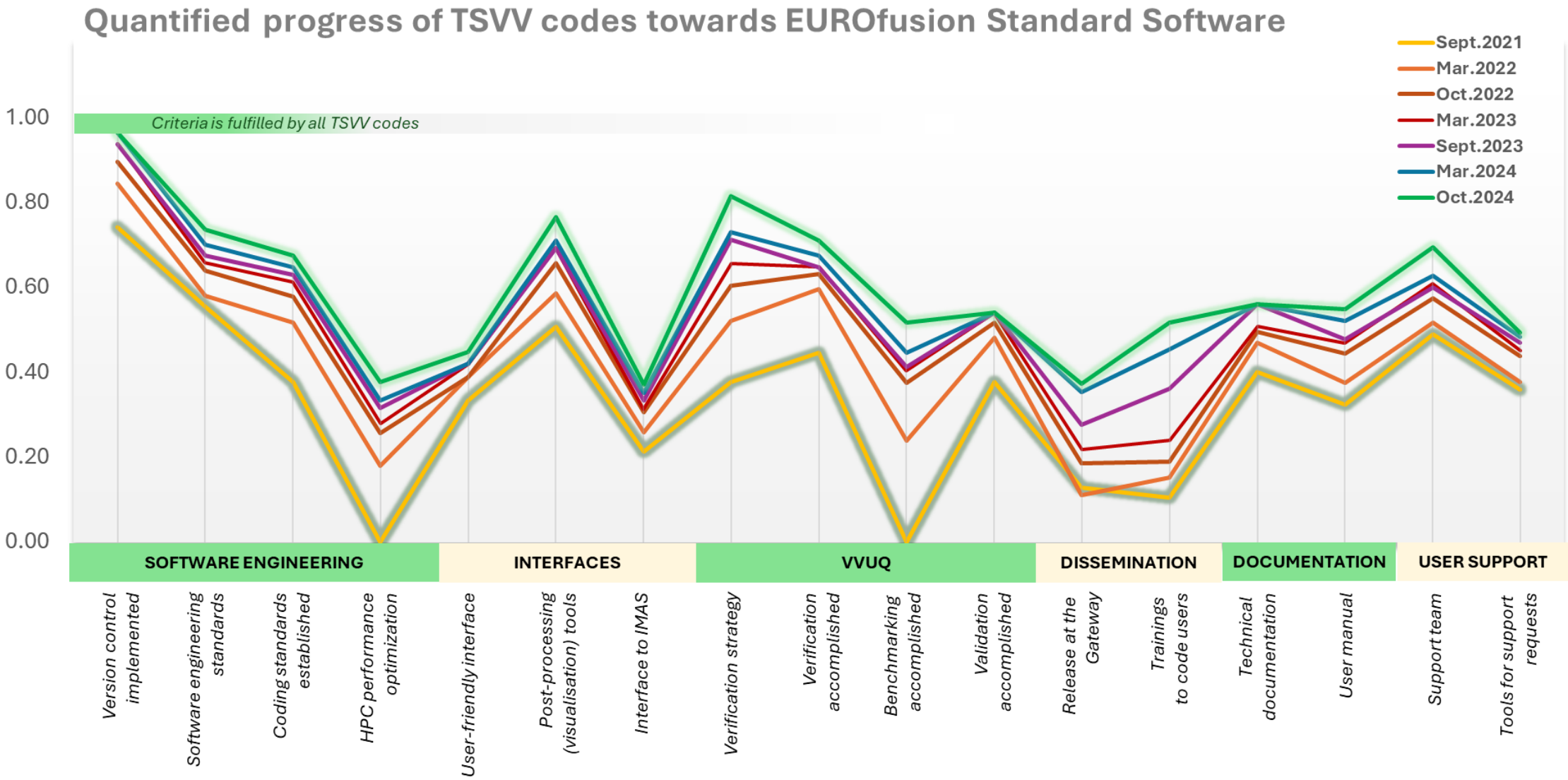
Addressed Stakeholders	Recommendations
Overall	• Ensure the availability of the urgently needed **Long-Term Data Storage Facility**. • Allocate **adequate resources for travel support** to enable closer collaboration among code developers and ACH members. • Ensure the advancement of expertise within the ACH teams by investing in **training and professional development** programs. • Explore pathways to supporting **an HPC/AI Summer School**.
EUROfusion PMU	• Set up a **central E-TASC website** to enhance communication. • Establish an **E-TASC online collaboration platform** to continuously share best practices and provide fast support for ongoing projects. • Organize **(bi-)annual in-person workshops between all E-TASC stakeholders** focused on networking and strategic planning.
ACH Coordinators	• Expand the ACH expertise in **database development**, particularly to manage large data sets and support the Data Management Plan. • Develop more competences in **AI/ML methods** to leverage these techniques for data validation, analysis, and optimization. • For HPC-oriented hubs, expand the competencies to effectively adapt to the **evolution in HPC hardware & software**. • Accelerate the development of the agreed-upon standards for the EUROfusion software stack by promoting **professional software engineering practices**. • Play a proactive role in proposing **projects of general interest**, in close collaboration with TSVVs, Thrusts, and WPs.
Code Developers	• Engage proactively with ACHs in a **one-team approach**. • Further strengthen the involvement of **ACH members in the research activities** (incl. co-authorships). • Commit sufficient **resources to support the ACH requests**. • Define **clear objectives and requirements** for each request. • Align your activities with the recommendations of the TSVV Mid-Term Review; this includes, in particular, the completion of the IMASification and the dissemination of the developed tools.

Towards EUROfusion Standard Software

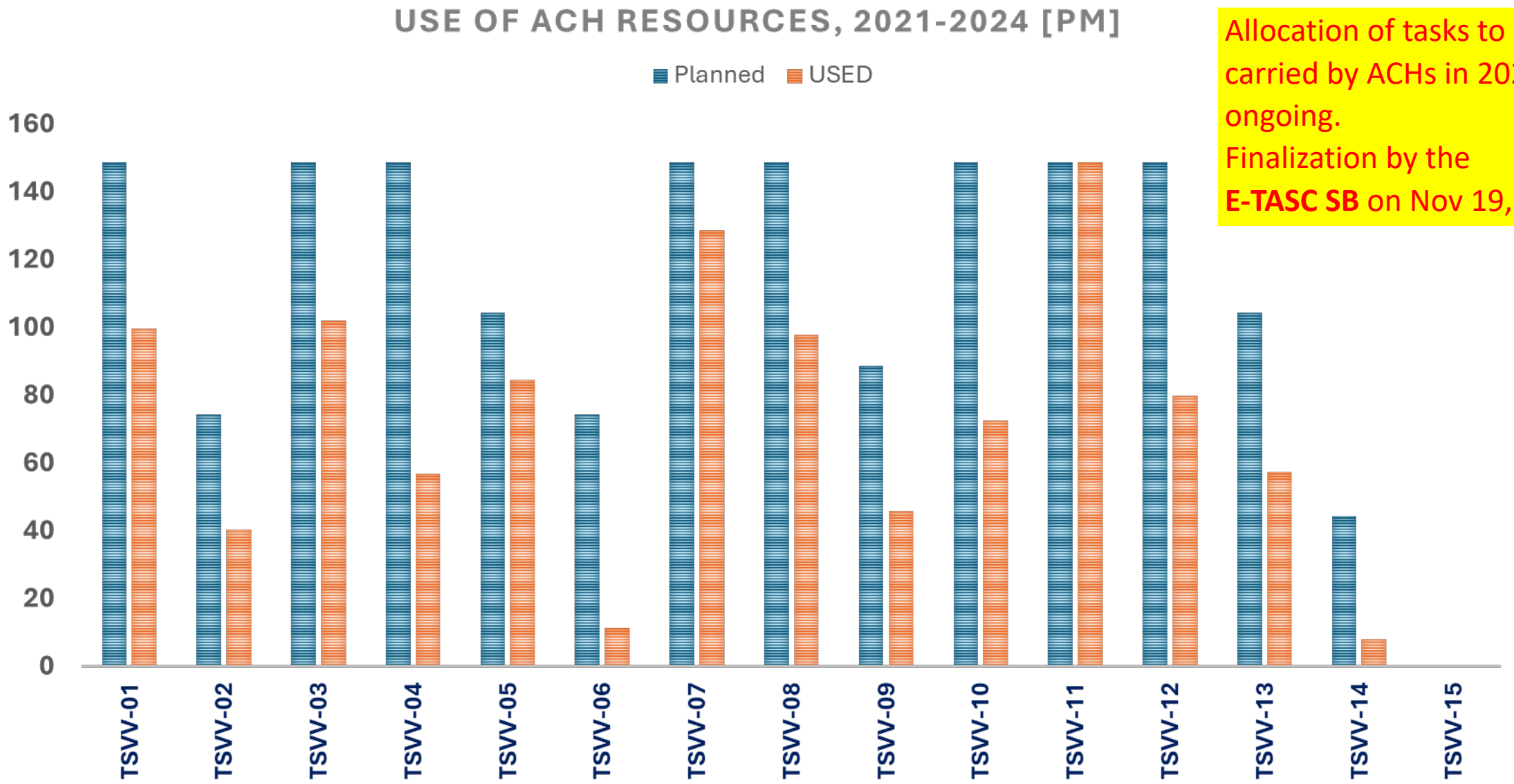
EUROfusion standard software will be developed with a very rigorous, consistent quality assurance process that is common across the E-TASC initiative; it is designed to benefit a wide range of users across EUROfusion, well beyond the team of code developers, and will adhere to the following guidelines and criteria:

- Free availability (within EUROfusion) of an up-to-date release version of the source code used for production runs
- Good software engineering practices (version control, regression/unit testing, shared development rules etc.)
- High-quality code documentation via user manuals and reference publications (including, in particular, a detailed description of the underlying model)
- Excellent support of users, co-developers, and support staff within EUROfusion (via contact person, mailing list, issue tracker, and the like)
- Specific plans for code verification and validation (involving a third party), in particular within EUROfusion, including aspects of uncertainty quantification
- User-friendly, intuitive interfaces and visualisation/post-processing tools, including interfaces to the IMAS Data Dictionary (where applicable)
- Specific plans for code dissemination and user training within EUROfusion

Progress towards EUROfusion Standard Software



Advanced Computing Hubs (cont'd)



Allocation of tasks to be carried by ACHs in 2025 is ongoing.
Finalization by the **E-TASC SB** on Nov 19, 2024

High Performance Computer and the Gateway cluster

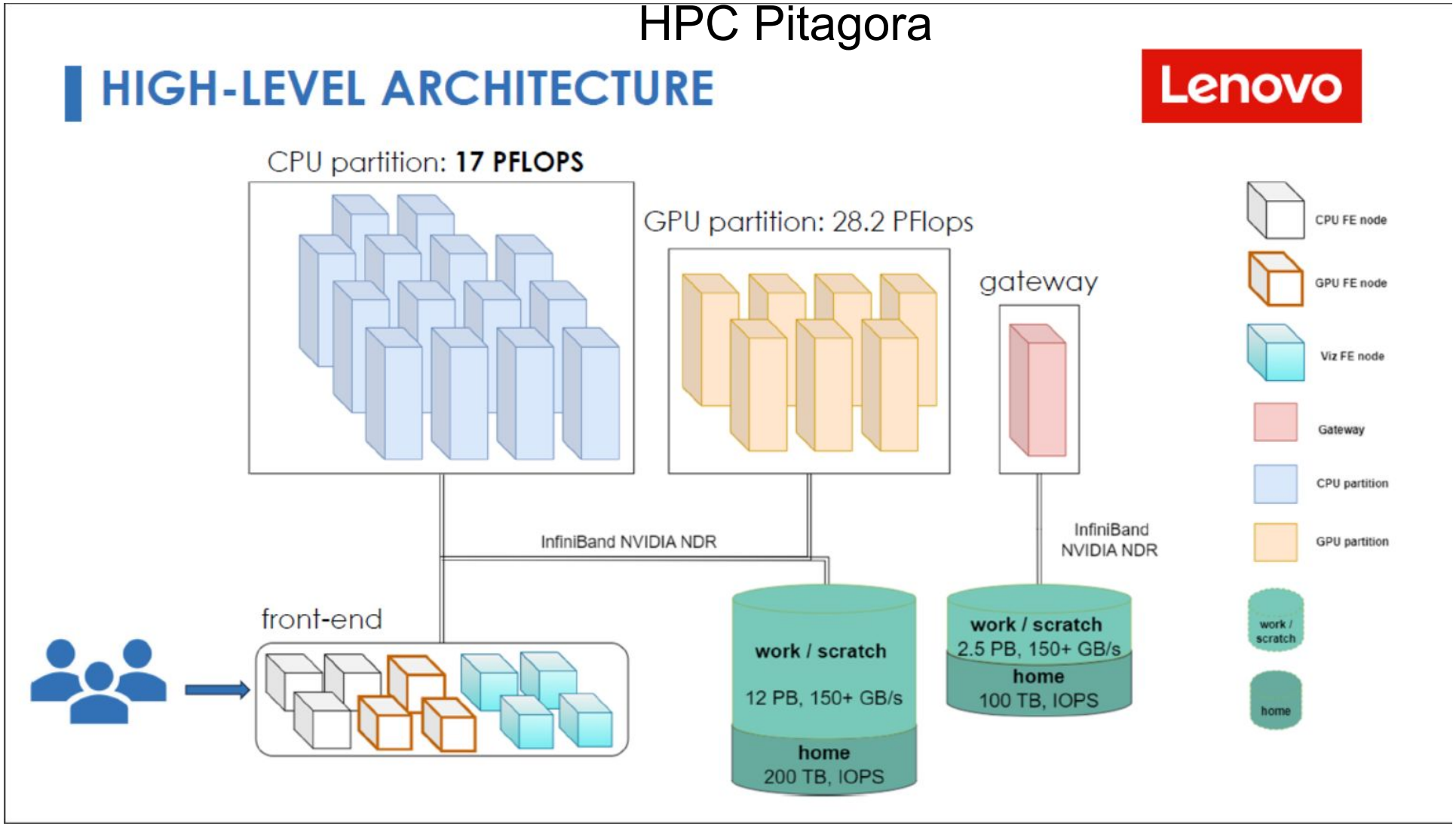
- The provision of computational resources to accommodate simulations in the context of activities within the WPs will be primarily done using the new:
  - **HPC infrastructure** (PITGORA, composed of a 17 Pflop/s CPU partition and a 28.2 Pflop/s GPU partition)
  - **Gateway cluster**
- The **new systems are expected to enter operation in late 2024 or early 2025**, following acceptance tests conducted by ACHs under the supervision of the HPC Operations Committee that will also monitor the operation to ensure high reliability and availability of the systems to the users throughout the year.
- A **target monthly availability of the systems of ≥ 97%** as in place for Marconi-Fusion and Leonardo in 2024 will be pursued.
- The allocation of HPC resources for cycle 9 of production runs in 2025 will take advantage of a 10x increase to fulfil requests from an expected similar number of projects (100+) as in 2024.

HPC resources for EUROfusion users in 2025

Progressive entry in operation of Pitagora as of Dec 2024

Marconi & Leonardo to be kept in operation to avoid gap

Few months overlap of Pitagora, Marconi & Leonardo



Implementation of the Data Management Plan (DMP)

Goal is to provide FAIR based data for EUROfusion experimental and simulation data (related to Grant deliverable)

Progress and issues in 2024

- Core services at PSNC/Gateway and participating sites [AUG, COMPASS, MAST/MAST-U, TCV, WEST and JET (JDC - 2024)]
  - Demonstrated remote data access through IMAS-based tools and protocols (UDA client server solution)
  - Security layer in UDA has been delivered, migration towards JSON plugin for simplified data mappings started on several sites
- Population of metadata catalog ready for production use, awaiting new Gateway hardware; demonstrated at SOFT 2024 (”scenario A”)
- IMASification of machine data → more resources and ability to move faster on data access (lack of expertise!)
- Demonstrated ability to provide data access for user driven application needs by running a predictive transport code (ETS) for AUG, WEST, [TCV,] and ITER on DMP provided data and access tools. (”scenario B”)
  - Expanded use requires Authentication and Authorisation technology to be further established at all sites
  - Reponsibility/willingness/ability to provide higher level data (core profiles etc) varies between sites – need an harmonized approach

Objectives for 2025

- Release production version of catalog for searchable metadata (waveforms) for all participating sites on the new Gateway
  - Finalize automation (new data ingested as they come available) and focus on performance optimisation and content amendments based on user requirements.
- Move towards providing data for user applications as a production service (TSVV codes and users)
  - Toolset in place, but data authorisation need to be rolled out
  - Data mappings need to be developed for specific use cases [interpretative/predictive modelling, MHD stability etc. (TSVV-01/10/11 etc.)
- Develop the technology to integrate modelling data through SimDB as a site (facility) of its own

New activities (implementation will depend on available resources)

Long Term Data Storage Facility (LTDSF)

- The simulation data produced by fusion research grows exponentially and gets more valuable as it represents spend computational time, and EUROfusion needs to secure long-term storage for such data.
- The storage solution shall be accessible for a minimum of 10 years, with provisions for expansion based on increasing data requirements.

Digital Twins

- The development of digital twins must be adopted to enable comprehensive, fully integrated simulations. These simulations should span various levels of abstraction, complexity, and reliability, encompassing not just the plasma itself but also external systems, control actuators, wall interfaces, and other engineering functionalities.
- In 2025 DSD is planning to start implementing several Proof of Concept (POC) projects that tie data from engineering and science together and will be defined answering to the needs and possibilities identified in a gap analysis.

Artificial Intelligence & Machine Learning (AI & ML)

- After a set of pilot projects has been implemented in various WPs in 2024, the next step might be to consolidate these efforts by increasing support of the most advances projects (according to the project review in early 2025) and by introducing an additional ACH focused on AI & ML.
- The effective training of AI tools will require a high-speed connection between the LTDSF, HPC, and Gateway.

E-TASC General Meeting (Nov 11-15, 2024)

Plenary Session 1: Research gaps and opportunities in simulation / theory
- Perspective of the Plasma Science Department (Marco Wischmeier)
- Perspective of the DEMO Central Team (Hartmut Zohm)
- Simulation and Theory in the USA (Michael Halfmoon)
- Simulation and Theory in the UK (Andy Davis)

Plenary Session 2: Status and plans of the TSVVs
- Overview talk (Frank Jenko)
- Poster session (TSVV coordinators)

Breakout sessions:
- PSD clarifications
- DEMO clarifications
- UK initiatives
- DMP use cases demo
- ITER clarifications
- Benefits of open science and open source software
- EUROfusion strategy for integrated modelling tools
- Round table discussion for TSVV PIs
- Round table discussion for ACH PIs

Details and registration:

https://indico.euro-fusion.org/event/3034

As of today: 78 registrations

Plenary Session 3: E-TASC and DSD beyond 2025
- DSD — present and future (Volker Naulin)
- E-TASC — present and future (Frank Jenko)
- Update on the Data Management Plan (Par Strand)
- Guided discussion: Further development of the TSVV-ACH ecosystem
- ITER-related research gaps (Simon Pinches)
- Guided discussion: Closing research gaps (incl. engineering & materials)

Plenary Session 4: Code dissemination
- Existing examples within EUROfusion (various speakers)
- Guided discussion: Building user communities & Practical implementation

Plenary Session 5: Towards EUROfusion Standard Software
- Motivation, criteria, progress, and challenges (Frank Jenko)
- Steps forward and the role of ACHs (Mervi Mantsinen)

Some thoughts on the E-TASC / DSD future

- The ideas presented by V. Naulin still **need to be discussed with the E-TASC Scientific Board**.
- New management positions should always be linked to **tangible added value**.
- **E-TASC has been operating very successfully so far**; the hybrid top-down and bottom-up approach is fruitful, and the E-TASC SB is highly agile.
- An **update of the TSVV ecosystem for 2026-27** is warranted, and the continuation of the ACHs is recommended.
- A key task for E-TASC in 2026-27 will be the **dissemination and expanded application of the newly developed simulation tools within the WPs**.