E-TASC General Meeting: E-TASC – Present and Future

Garching| Nov 11-15, 2024

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On behalf of the E-TASC SB

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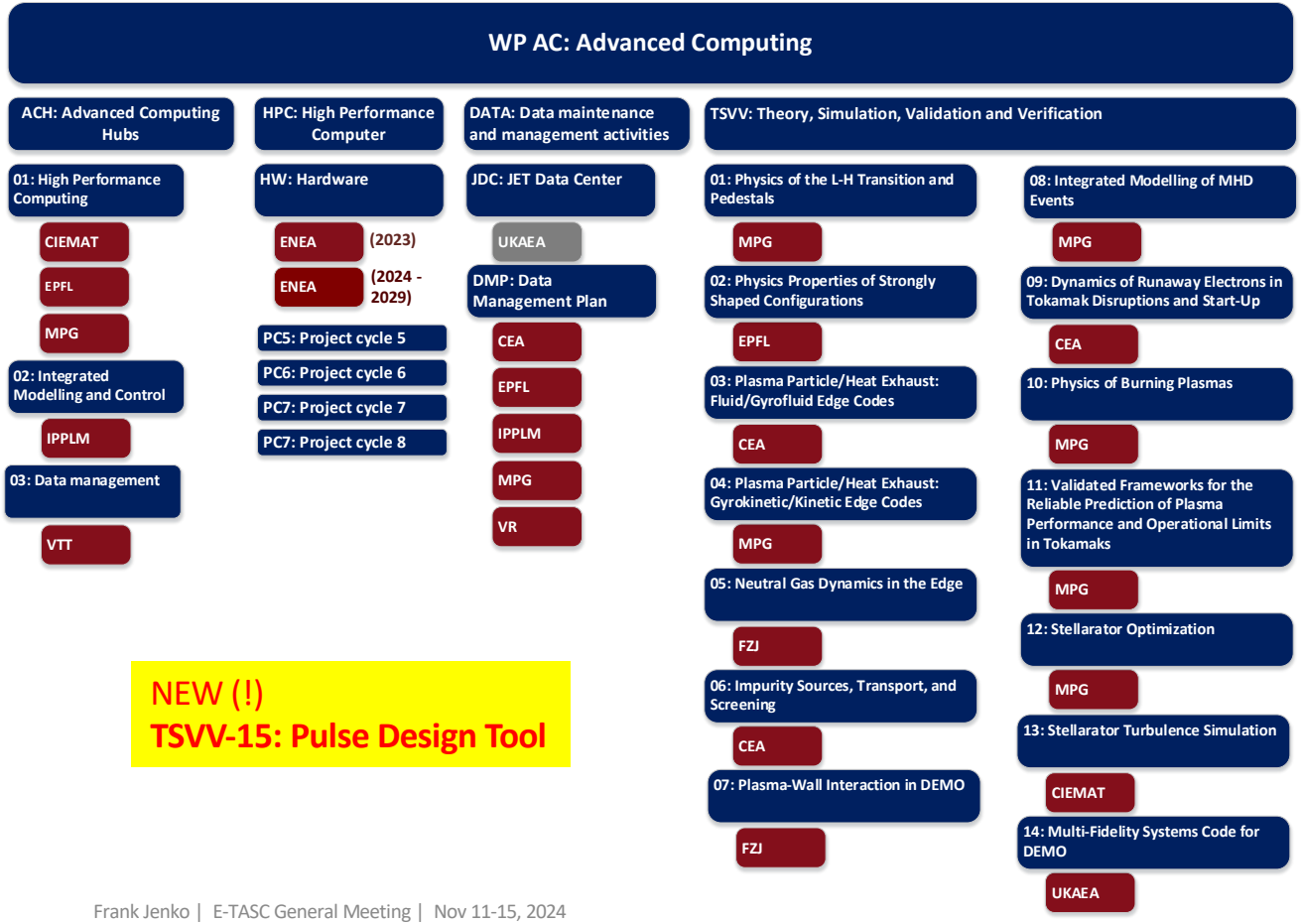
E-TASC within the WP Advanced Computing



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/

Mid-term review: Summary of key action items

Providing resources for strengthening collaborations and enabling trainings within the E-TASC ecosystem

- A concrete travel budget proposal will be discussed at the next FSD Project Board meeting

Increased focus on the development of EUROfusion Standard Software

- More emphasis on cross-code fertilization, the completion of the IMASification, and the dissemination of the developed tools (incl. code documentation, code repositories, user training etc.)

Enabling modern data-driven plasma science

- In this context, the E-TASC SB fully supports the recent call for "Project proposals for innovative AI/ML methods used in support of EUROfusion programme objectives"
- Additional action items should include manned support for FAIR access to all EU tokamak databases in IMAS format and the acquisition of a long-term storage facility for simulation databases

Software licensing

- A clear recommendation on licenses (or license options) to be used should be provided on a EUROfusion-wide basis in a timely fashion; a subgroup of the E-TASC SB has agreed to put together a specific proposal

Development of a Pulse Design Tool (PDT)

- Recently, a small new activity (embedded in TSVV-11) has been launched by the PMU to identify possible paths forward regarding the development of a PDT by the end of the year
- The SB and several TSVV leaders will play an active role in this context

ACH selection & monitoring (by E-TASC SB)

Call: Spring 2020

EUROfusion

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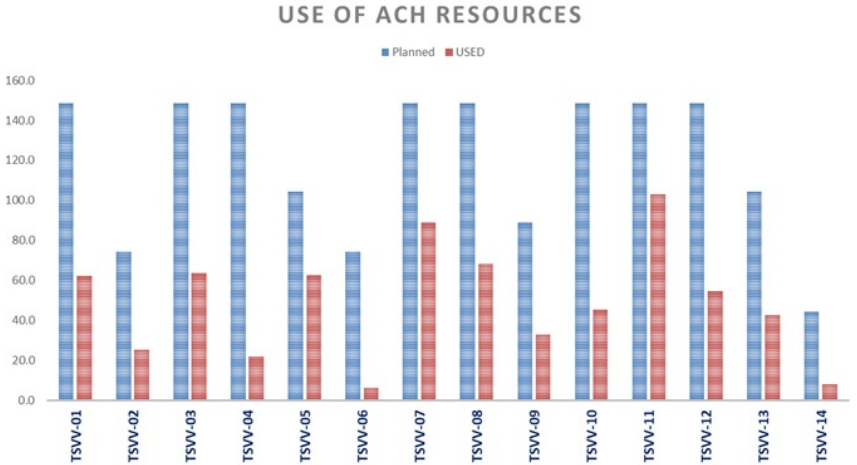
Our ref: PMU/1740

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 Coordin	PM's requested	PM's assigned	ACH team members	Tasks description	Comments
2021	EPFL	TSVV-13	EUTERPE		2,0	0,5	Lanti	Further development of GPU functionality (OpenACC) for large-scale EM turbulence simulations.	
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	
2021	EPFL	TSVV-03	FELTOR		1,5	0,5			task distributed per code
2021	EPFL	TSVV-03	GBS		1,5	0,5			task distributed per code
2021	EPFL	TSVV-03	GBS		1,2	1,0	Lanti	Optimization of kinetic neutrals treatment (method of characteristics and coupling to EIRENE)	
2021	EPFL	TSVV-03	GBS		6,0	1,0	Peytavmes/Vaimi	Code profiling and optimization	
2021	EPFL	TSVV-03	GRILLIX		1,5	0,5			task distributed per code
2021	EPFL	TSVV-03	GRILLIX		6,0	1,0	Peytavmes/Vaimi	Code profiling and optimization	
2021	EPFL	TSVV-01	GYSELA		1,5	1,0	Peytavmes	Support for GPU porting and increased vectorisation for ARM-based architectures	
2021	EPFL	TSVV-04	GYSELA		1,5	1,0	Peytavmes	Support for GPU porting and increased vectorisation for ARM-based architectures	
2021	EPFL	ACH	management	Paolo Ricci	1,5	1,5	Paolo Ricci	management of ACH activities	
2021	EPFL	TSVV-01	ORB5		4,0	1,0	Lanti	Improve multi-threading of ORB5 & particularly of its field solver. Adaptations to the M100	
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	
2021	EPFL	TSVV-03	ORB5		4,0	1,0	Lanti	Further development of GPU functionality (OpenACC) for large-scale EM turbulence simulations.	task distributed per code
2021	EPFL	TSVV-13	ORB5		2,0	0,5	Lanti	Further development of GPU functionality (OpenACC) for large-scale EM turbulence simulations.	task distributed per code
2021	EPFL	TSVV-03	SOLEDGE3X		1,5	0,5	Vaimi	Poisson solver optimization, including porting to GPU	
2021	EPFL	TSVV-06	SOLEDGE3X		3,0	1,0	Peytavmes/Vaimi	Profiling and optimisation of SOLEDGE3X in the case of high number of species	
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	
2021	IPPLM	ALL	AAI	Lluiz Jolia	5,0	5,0	Pawel Spychala	AAI Infrastructure Rollout and support	
2021	IPPLM	TSVV-12	ASCOTS	Per	0,5	0,3	Michal Poradzinski	ASCOTS. Implementation in IMAS framework	
2021	IPPLM	TSVV-12	BEAMS3D	Per	0,5	0,3	Michal Poradzinski	BEAMS3D. Implementation in IMAS framework	
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	
2021	IPPLM	TSVV-03	DATABASE5	Patrick	6,0	2,5	Daniel Figat	This task is led by VTT ACH. We can help with the Repository and Continuous Integration	
2021	IPPLM	TSVV-11	DATABASE5	Clarisse	3,0	1,0	Dimitriy Yadykin	Initial implementation of multimachine remote data gathering and (for 1D profiles) fitting using	
2021	IPPLM	ALL	DEVOPS	Clarisse	2,4	2,0	Daniel Figat	Aid with setup and maintenance of potential new DevOps platform and documentation. To be	
2021	IPPLM	TSVV-09	DREAM	Eric Nardon	6,0	0,5	Dimitriy Yadykin	DREAM integration into IMAS	
2021	IPPLM	TSVV-11	DYON	Clarisse	1,2	0,3	Michal Owsiak	Adapt DYON to IMAS and containerise (and adapt from matlab to octave or python)	
2021	IPPLM	TSVV-05	EIRENE	Dmitry	0,5	0,2	Dimitriy Yadykin	Integration of code I/O in the IMAS	
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	
2021	IPPLM	ALL	ETS	Per Strand	3,5	3,5	Per Strand	ACH-workflows/ETS	
2021	IPPLM	TSVV-03	FELTOR		1,5	0,1			task distributed per code
2021	IPPLM	TSVV-03	GBS		1,5	0,1			task distributed per code
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)	
2021	IPPLM	TSVV-03	GRILLIX		1,5	0,1			task distributed per code
2021	IPPLM	TSVV-11	HPPS	Clarisse	3,0	3,0	Bartosz Bosak	Containerise HCD workflow (Docker)	
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	
2021	IPPLM	TSVV-11	HPPS	Clarisse	1,8	1,0	Bartek Palak	Adapt existing HPPS python components from FC2K to hetsp	
2021	IPPLM	TSVV-11	HPPS	Clarisse	2,4	2,0	Daniel Figat	Setup common IMAS-python workflow testing framework. Add CI build and run tests for HPPS	
2021	IPPLM	TSVV-11	HPPS	Clarisse	3,0	2,0	Bartek Palak	Adapt existing Kepler based components to IMAS Python workflows and hetsp	
2021	IPPLM	TSVV-11	HPPS	Clarisse	0,6	0,6	Dimitriy Yadykin	Provide SOL models (as in Lucia NP2020 for example) parameterisation as a simple IMAS python	
2021	IPPLM	ALL	IMAS	Marcin	8,0	8,0	Marcin Plociennik	IMAS Ecosystem Infrastructure support+maintenance+deployments	
2021	IPPLM	TSVV-01	IMAS	Tobias	1,0	0,3	Michal Owsiak	IMAS code output support/training	
2021	IPPLM	TSVV-10	IMAS	Oleksiy	2,0	2,0	Per Strand	Up-to-date IMAS support including ITER/WPCD integrated modeling tools, experimental data	
2021	IPPLM	TSVV-11	IMAS	Clarisse	1,2	1,0	Tomasz Zok	Design python IMAS workflows for multiple containers, use JINTRAC+H2D as template / proof of	
2021	IPPLM	TSVV-11	IMAS	Clarisse	1,2	1,0	Bartosz Bosak	Containerise NICE (Docker)	

Recommendations (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 and 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.

Recommendations (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.

Recommendations (EUROfusion PMU)

Set up a **central E-TASC website** to enhance communication.

- This **will complement existing websites** for the individual TSVVs.

Establish an **E-TASC online collaboration platform** to continuously share best practices and provide fast support for ongoing projects.

- ACH@Poznan has access to and experience with various tools.
- They will reach out to the other ACHs and **propose a specific solution before the end of July**.

Organize **(bi-)annual in-person workshops between all E-TASC stakeholders** focused on networking and strategic planning.

- E-TASC General Meeting will take place on November 11-15, 2024.
- This will be the **first in-person meeting of all stakeholders** – after almost 4 years.
- Strategic planning will play a key role.

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.

- As of now, each ACH / TSVV has about 3k€ / 5k€ per year (~50% of what was asked for).
- We are getting many requests; **a budget increase would be extremely helpful**.

Ensure the advancement of expertise within the ACH teams by investing in **training and professional development programs**.

- Key aspect for attracting, retaining, and equipping high-quality personnel.
- We will invite **experts from neighboring areas of R&D** for webinars and visits.

Explore pathways to supporting an **HPC/AI Summer School**.

- Successful example: Computational Physics School for Fusion Research (MIT)
- We could **partner with European supercomputing centers, CERN, and FuseNet**.

Evolution of the TSVV / ACH ecosystem in 2026-27

Main tasks:

- **Code development** (in collaboration with ACHs)
- **Code validation & applications** (with WPs)
- **Code deployment** (including user training and support)

Prerequisites for code support:

- **Appropriate data environment (including IMAS integration)**
- **Open access for the EUROfusion community**

Implications:

- Existing TSVVs are expected to evolve and possibly merge
- New pilot TSVVs in fusion engineering and technology
- Potential adjustments in ACH responsibilities