EUROfusion
FUSION SCIENCE DEPARTMENT

# WPAC 2022 Scientific Goals

*FSD Science Coordination Meeting in Preparation for 2022*

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**With Volker Naulin and Denis Kalupin**
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# Activities included in the WP Advanced Computing

TSVV

**…coordination** is required that can integrate the world-class fusion science and engineering with emerging advanced computing capabilities – this is the vision for E-TASC, which stands for the EUROfusion – Theory and Advanced Simulation Coordination, (EUROFUSION GA (18) 24 - 4.6 and see also Chapter 2) which is implemented under WP AC.

A set of TSVV tasks are established, with **connection to relevant Work Packages** as listed in this chapter.

ACH

The ACHs will provide essential expertise and support in computer science, scientific computing, data management, code integration, and software engineering, as well as in the development of a suitable portfolio of **EUROfusion standard software codes**.

JDC

**JET Data Centre** as a long term hub to maintain JET experimental data.

HPC

… the **procurement, installation, operation and upgrade of HPC resources for the EUROfusion programme**. Currently this programme relies on access to a dedicated part of the MARCONI supercomputer, funded by EUROfusion FP8 and operated by CINECA in Bologna with 10 PFlops peak dedicated to EUROfusion in its present phase (2019-2023).

# Work Breakdown Structure

**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**
  - TBD
- **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

WBS of the WP AC follows the **activity** / **project** structure

The implementation of ACH and TSVV areas are following the project selection recommended by the **E-TASC SB** and endorsed by **EUROFUSION GA (21) 33**.

Implementation of other areas is postponed until the selection of beneficiaries that will be providing relevant services is done.

(Provisional timing:
for **JDC – end of 2021**;
for **HPC – middle of 2023**)

# List of endorsed TSVV projects and ACHs

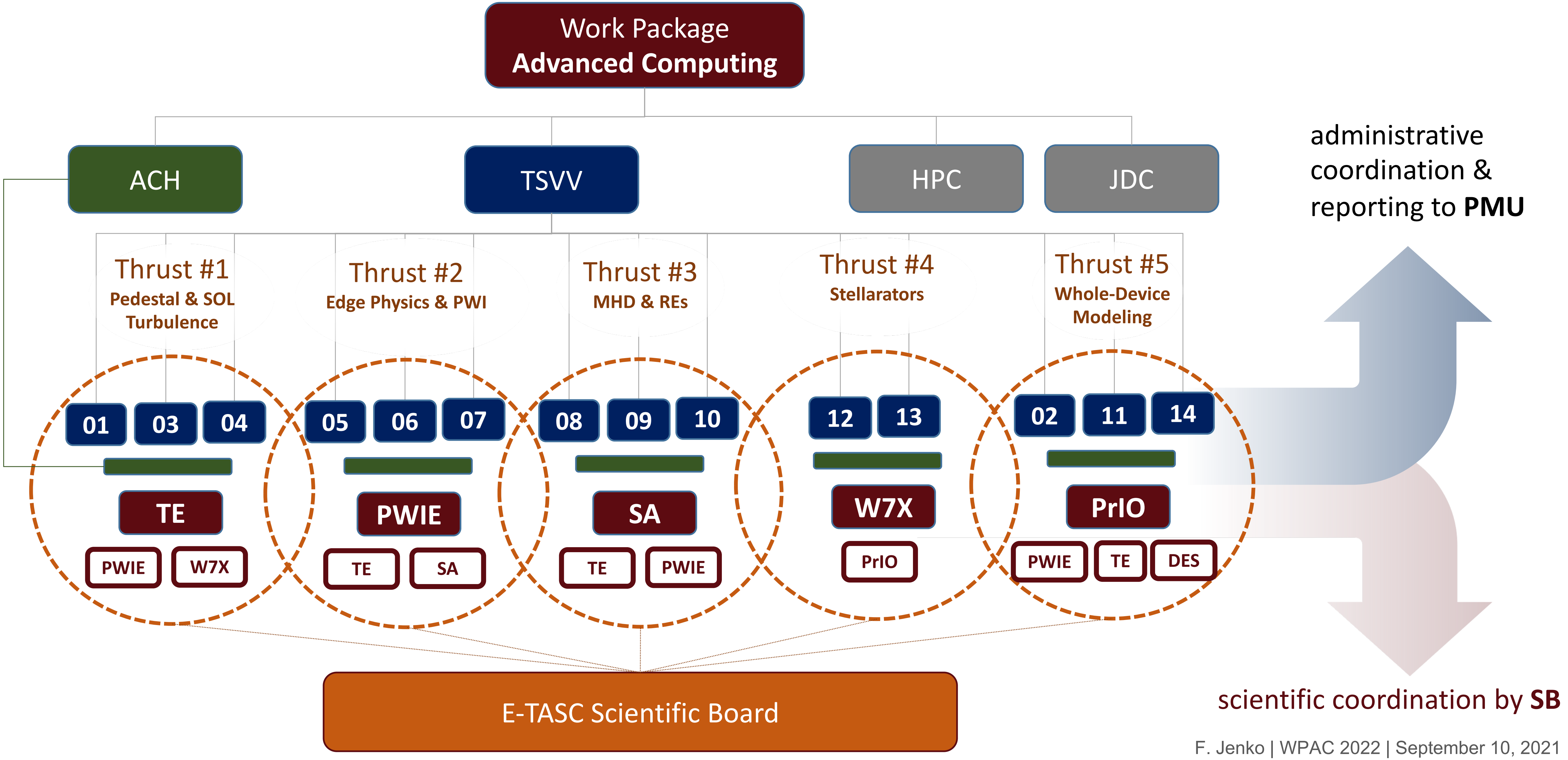
## TSVV

| TSVV No | Lead Beneficiary | Principal Investigator | Title |
|---|---|---|---|
| 1 | MPG | Tobias Görler | Physics of the L-H Transition and Pedestals |
| 2 | EPFL | Justin Ball | Physics Properties of Strongly Shaped Configurations |
| 3 | CEA | Patrick Tamain | European boundary plasma modelling towards reactor relevant simulations |
| 4 | MPG | Daniel Told | Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes |
| 5 | FZJ | Dmitriy Borodin | Neutral Gas Dynamics in the Edge |
| 6 | CEA | Guido Ciraolo | Impurity Sources, Transport, and Screening |
| 7 | FZJ | Dmitry Matveev | Plasma-Wall Interaction in DEMO |
| 8 | MPG | Matthias Hölzl | Integrated Modelling of Transient MHD Events |
| 9 | CEA | Eric Nardon | Dynamics of Runaway Electrons in Tokamak Disruptions |
| 10 | MPG | Oleksiy Mishchenko | Physics of Burning Plasmas |
| 11 | CEA | Clarisse Bourdelle | Validated frameworks for the Reliable Prediction of Plasma Performance and |
| 12 | MPG | Per Helander | Stellarator Optimization |
| 13 | CIEMAT | Jose Manuel Garcia Regana | Stellarator Turbulence Simulation |
| 14 | CCFE | James Morris | Multi-Fidelity Systems Code for DEMO |

## ACH

| ACH Cat. | Lead Beneficiary | Principal Investigator | Category Title |
|---|---|---|---|
| 1 | MPG | Roman Hatzky | **High Performance Computing** (scalable algorithms, code parallelization & performance optimization, code refactoring, GPU-enabling etc.) |
| 1 | EPFL | Paolo Ricci | **High Performance Computing** (scalable algorithms, code parallelization & performance optimization, code refactoring, GPU-enabling etc.) |
| 1 | CIEMAT | Mervi Mantsinen | **High Performance Computing** (scalable algorithms, code parallelization & performance optimization, code refactoring, GPU-enabling etc.) |
| 2 | IPPLM | Marcin Plociennik | **Integrated Modelling and Control** (code adaptation to IMAS, IMAS framework development, code integration etc.) |
| 3 | VTT | Fredric Granberg | **Data management** (open access, data management, data analysis tools, aspects of AI and VVUQ etc.) |

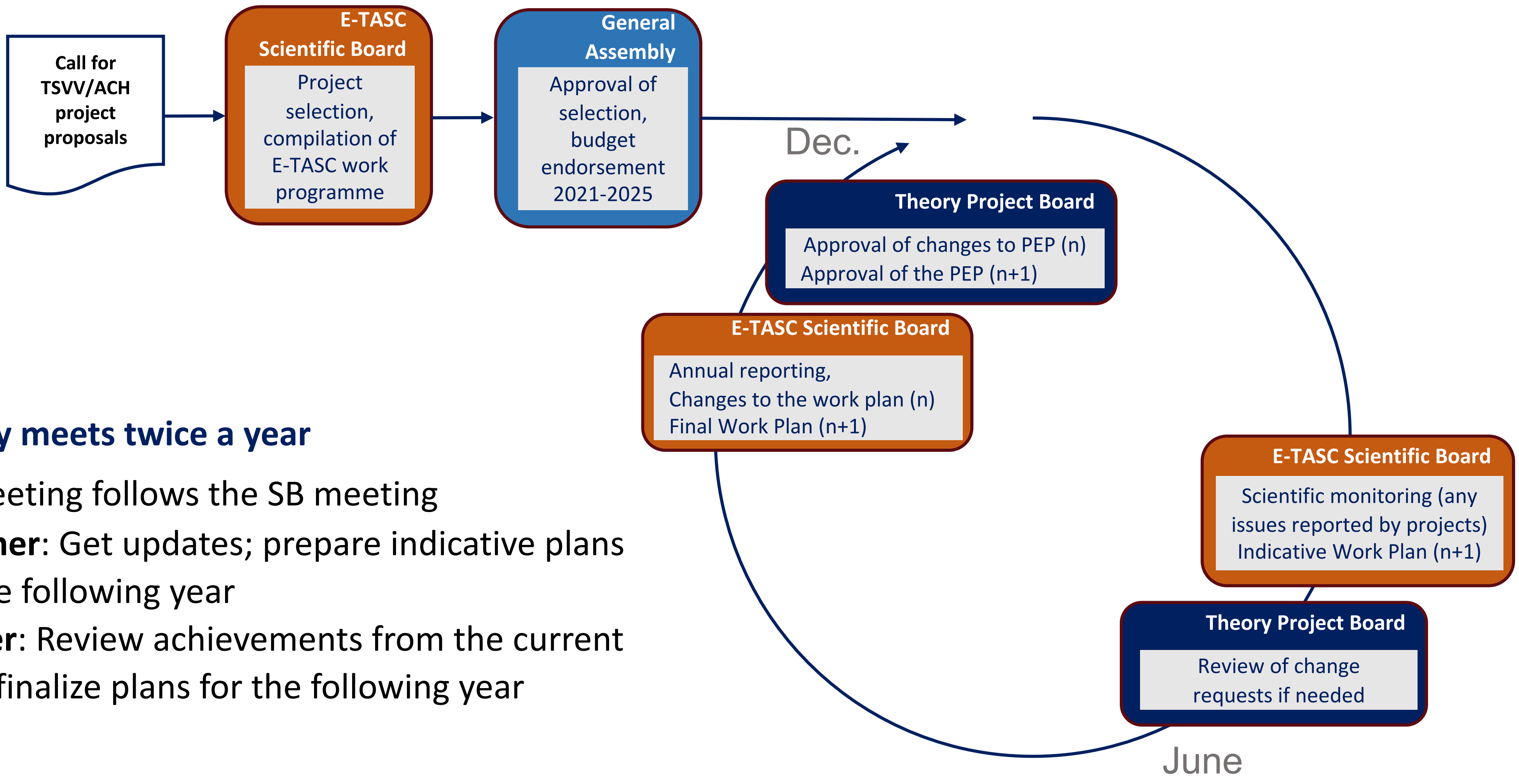
# Interactions with other WPs



# Roles and Responsibilities

| Organization name | Stakeholder name | Main role and responsibilities |
|---|---|---|
| **TSVV / ACH** | **Principal Investigator** | The PI of a TSVV/ACH is responsible for the implementation and reporting of its activities in line with the work programme recommended by the E-TASC SB and formally approved with resources by the Theory PB. The PI acts as the endorser of publications produced by the TSVV/ACH, together with the involved WP's PLs or TFLs. |
| **Thrust** | **Facilitator**<br><br>Project Leader (also TFL for campaign oriented WPs) | A Thrust serves as a **communication platform** among a group of related TSVVs and WPs, on behalf of the entire E-TASC SB. It consists of a set of TSVV leaders, E-TASC SB members, and relevant PLs/TFLs and is coordinated by a facilitator chosen among the latter. The facilitator provides feedback on the Thrust activities and proposes corrective actions for the TSVV work programmes to the E-TASC SB if and when needed. **Joint validation efforts, open physics problems, new tools…** |
| **E-TASC SB** | **Scientific Board** (appointed by the Programme Manager) | The E-TASC SB is an advisory body, acting in pursuit of the overall success of the E-TASC initiative. The E-TASC SB advises the Programme Manager on the selection and continuation of TSVVs and ACHs. It develops a coherent TSVV/ACH scientific programme through specific tasks, milestones, and deliverables and to establishing a close interaction between all TSVVs and ACHs. It ensures that TSVVs/ACHs are progressing according to the agreed plans, reviews the reports from the TSVV/ACH PIs, and recommends corrective actions for the approval of the Theory PB if and when necessary. |
| **Theory PB** | **Project Board** (appointed by the Programme Manager) | The Project Board supports the PIs of TSVVs/ACHs in their efforts on the basis of E-TASC SB recommendations, approves the resources and annual work programme of the WP AC and WP EnR (Inertial Fusion and Theory & Modelling areas), and resolves possible conflicts between stakeholders. |
| **PMU** | **FSD Department** | The PMU supports the PIs of TSVVs/ACHs in their efforts, fosters communication between all involved stakeholders, and ensures that all E-TASC activities are aligned with the programmatic objectives of EUROfusion. |

# SB – PB interactions




## Each body meets twice a year

– PB meeting follows the SB meeting
– **Summer**: Get updates; prepare indicative plans for the following year
– **Winter**: Review achievements from the current year; finalize plans for the following year

# Work Programme 2021/22

*14 TSVV Tasks, grouped in 5 Thrusts*

# Work Programme 2021/22 – Thrust 1: Pedestal & SOL Turbulence

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

- 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 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.

**TSVV Task 3: Plasma Particle/Heat Exhaust: Fluid/Gyrofluid Edge Codes**

- Develop a comprehensive modelling capability (incl. anomalous transport) for the plasma edge based on fluid/gyrofluid equations, ideally including important kinetic effects and a realistic description of plasma-wall interactions.
- Ensure that the respective tools exhibit good scalability on high-performance computers, such that reliable and accurate results can be obtained for the preparation and interpretation of experiments and the design of fusion power plants.
- Validate these tools and apply to address key physics questions.

**TSVV Task 4: Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes**

- Capability to predict the plasma particle/heat exhaust on the basis of GK and FK approaches, in conditions pertinent to a collisional plasma edge/SOL; exploit synergies with TSVV Task 1.
- Systematic investigation of the limitations of GK theory in edge/SOL conditions.
- Construct methodologies to couple FK and GK approaches, as well as GK and fluid/gyrofluid approaches.

# Work Programme 2021/22 – Thrust 2: Edge Physics & PWI

**TSVV Task 5: Neutral Gas Dynamics in the Edge**

- Development of a state-of-the-art neutral gas code towards optimal scalability on high-performance computing systems.
- Establishment of a multi-fidelity model hierarchy for the neutral gas phase in fusion devices; from first principles towards reduced models. Validation of the established models.
- Enabling model reduction and improved code-code coupling towards model integration (via IMAS). Provision of a neutral gas code as input to existing and future plasma boundary codes for ITER, W7-X, DEMO etc. (see TSVV Tasks 3 and 4).

**TSVV Task 6: Impurity Sources, Transport, and Screening**

- Establish an integrated modelling suite to predict the W impurity distribution in DEMO, including W source generation, W screening, W transport, W exhaust and its impact on the plasma performance.
- Develop 3D kinetic transport models for heavy impurities (including W) and seeding species like Ar, Kr, and Xe in the SOL and pedestal regions of DEMO.
- Assess the effects of 3D perturbations and ELM suppression techniques on the W impurity distribution in ITER reference scenarios, along with their implications for DEMO.

**TSVV Task 7: Plasma-Wall Interaction in DEMO**

- Establish an integrated modelling suite to predict steady-state PWI in DEMO.
- Provide safety-relevant information for DEMO reference scenarios concerning first-wall erosion, dust, and fuel inventory.
- Develop modelling capabilities to treat DEMO-relevant transients.

# Work Programme 2021/22 – Thrust 3: MHD and Runaway Electrons

**TSVV Task 8: Integrated Modelling of Transient MHD Events**

– Extend the capability of global nonlinear MHD modelling to capture MHD control techniques for the avoidance and mitigation of disruptions and ELMs.
– Provide capabilities to couple high-fidelity MHD modelling to existing or future integrated modelling tools.
– Establish a validated modelling hierarchy for MHD control suitable for real-time applications.

**TSVV Task 9: Dynamics of Runaway Electrons in Tokamak Disruptions**

– Provide a self-consistent, robust, and validated model for RE dynamics and mitigation in the presence of shattered pellet injection and 3D fields.
– Develop and validate a model for the RE beam generation and losses to be used within the integrated modelling tools and nonlinear MHD codes for accurate prediction of unmitigated and mitigated disruptions.

**TSVV Task 10: Physics of Burning Plasmas**

– Develop a self-consistent description of, and corresponding simulation tools for, the mutual interaction of energetic particles with MHD modes and turbulence, as well as their interplay with the kinetic plasma profiles in both tokamak and stellarator geometries.
– Develop a theoretical understanding and a validated interpretative/predictive capability of the physics of burning plasmas in both tokamak and stellarator geometries.
– Develop strategies to optimize the deposition of the fusion $\alpha$ energy to the bulk plasma (improved reactor performance).

# Work Programme 2021/22 – Thrust 4: Stellarators

## TSVV Task 12: Stellarator Optimization

- Develop a new, advanced European stellarator optimization code, based on improved algorithms for enhanced speed and greater scope.
- Generate a number of highly optimized stellarator configurations which could form the basis for future stellarator devices and support the decision on how to progress with a next-step stellarator device.

## TSVV Task 13: Stellarator Turbulence Simulation

- Develop, verify, and validate a set of Stellarator gyrokinetic codes going beyond the flux tube approach and self-consistently treating multiple particle species.
- Validate (and adapt, if needed) these codes for the calculation of turbulent fluxes in tokamaks with broken axisymmetry.
- Apply these codes (and theory) to enhance the basic understanding of micro-instabilities and turbulence in stellarators in different geometries and plasma conditions.

# Work Programme 2021/22 – Thrust 5: Whole-Device Modeling

**TSVV Task 2: Physics Properties of Strongly Shaped Configurations**

- Explain the effects of NT (and strong shaping in general) on plasma performance in terms of confinement, stability, and compatibility with highly radiative/dissipative scenarios.
- Extrapolate the results to a reactor-scale device and help identify the advantages and disadvantages w.r.t. PT concepts.

**TSVV Task 11: Validated Frameworks for the Reliable Prediction of Plasma Performance & Operational Limits in Tokamaks**

- Establish an integrated modelling framework (according to EUROfusion software standards) by coupling core and edge physics modules using validated, reliable models (involving predictive transport solvers) to enable the simulation of complete plasma operational scenarios from breakdown to termination under metallic wall conditions as on ITER/DEMO.
- Integrate and/or develop (if needed) state-of-the-art models for turbulent transport, pedestal and SOL physics, impurity transport, energetic particles transport, and stability of burning plasmas (ITER/DEMO operational regimes).
- The models & tools should be developed considering the input and feedback of users around existing machines, which will help improve them and, most importantly, ensure they will be ultimately used by the community.

**TSVV Task 14: Multi-Fidelity Systems Code for DEMO**

- Removal of computational bottlenecks in the analysis of DEMO systems.
- Automation of the generation of inputs to allow the cascade of modelling from low- to high-fidelity to be simplified.
- Implementation & validation of these models for physics/engineering systems to be integrated into a whole-plant model.
- Implementation of optimization methods for application to multi-fidelity multi-system modelling, and quantification of the propagation of uncertainties through the whole-plant model process.

# Work Programme 2021/22

*5 Advanced Computing Hubs*

# Matching TSVV needs with ACH expertise

An optimal allocation of the individual tasks requested by the TSVVs to the work skills and human resources of the ACHs is crucial for the overall success of E-TASC.

The selection process has been divided into several stages:

- Submission of proposals by the TSVV PIs (high-moderate-low priority)
- Individual assessment of the proposals by the ACH PIs (traffic light system)
- Joint coordination meeting of all ACH PIs
- Proposition of a 2021/22 work plan for each ACH
- Evaluation and approval by the E-TASC Scientific Board
- Approval by the Project Board Theory

# Collaborative spirit and flexibility

**Collaborative spirit**

- Many ongoing discussions between the various stakeholders (TSVVs, ACHs, WPs, SB)
- ACHs and TSVVs to establish *joint* efforts, with manpower investments on *both* sides
- A „throwing-the-code-over-the-fence“ approach is neither realistic nor desirable
- ACH members as integral part of the code development team, with tangible incentives

**Flexibility**

- Specific plans for 2021/22, but a project‘s scope/duration may need to be adapted
- Progress will be monitored by the E-TASC SB and reviewed at least twice per year
- Plans include some contingency
- Will be able to accommodate additional requests as the ACHs approach full operation (2023-)

# Work Programme 2021/22

*Note: The numbers in brackets indicate the involved TSVVs*

**ACH-CIEMAT** [Cat. I: HPC]
Codes: BIT1 (3), ERO2.0 (7), SPICE (7), KNOSSOS (12), STELLA (13), BLUEMIRA (14)

**ACH-EPFL** [Cat. I: HPC]
Codes: ORB5 (1/2/10), GBS/FELTOR/GRILLIX/SOLEDGE3X (3/6), ASCOT5 (12), CAS3D (12), GYSELA (1/4), EUTERPE (13)

**ACH-MPG** [Cat. I: HPC]
Codes: EIRENE (5), EUTERPE (10/13), GENE (1/4/13), GVEC (12), JOREK (8), VM2MAG (12)
General support for MARCONI

**ACH-IPPLM** [Cat. II: IM]
Substantial support for TSVV-11 (IM framework)
IMAS support for a wide range of codes (incl. JOREK)

**ACH-VTT** [Cat. III: DM]
Codes: EIRENE (5), GBS/FELTOR/GRILLIX/SOLEDGE3X (3), DREAM (9), QLKNN (11), BLUEMIRA (14) + materials science
Other activities: databases, data compression, VVUQ, AI/ML

# Some points for discussion

**After the first few months…**

- How did the first round of Thrust meetings go?
- Best practices: What does (or does not) work well so far?
- How to best interact across Thrusts?
- How to best link tokamak and stellarator efforts?
- Any other observations or suggestions?