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EUROfusion-theory and advanced simulation coordination (E-TASC): programme and the role of high performance computing

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Abstract

This paper is a written summary of an overview oral presentation given at the 1st Spanish Fusion High Performance Computer (HPC) Workshop that took place on the 27 November 2020 as an online event. Given that over the next few years ITER[24] will move to its operation phase and the European-DEMO design will be significantly advanced, the EUROfusion consortium has initiated a coordination effort in theory and advanced simulation to address some of the challenges of the fusion research in *Horizon EUROPE* (2021–2027), i.e. the next EU Framework Programme for Research and Technological Development. This initiative has been called E-TASC, which stands for EUROfusion-Theory and Advanced Simulation Coordination. The general and guiding principles of E-TASC are summarized in this paper. In addition, an overview of the scientific results obtained in the pilot phase (2019–2020) of E-TASC are provided while highlighting the importance of the required progress in computational methods and HPC techniques. In the initial phase, five pilot theory and simulation tasks were initiated: towards a validated predictive capability of the low to high transition and pedestal physics; runaway electrons in tokamak disruptions in the presence of massive material injection; fast code for the calculation of neoclassical toroidal viscosity in stellarators and tokamaks; development of a neutral gas kinetics modular code; European edge and boundary code for reactor-relevant devices. In this paper, we report on recent progress made by each of these projects.

Keywords: theory and simulation, high performance computer, EUROfusion

(Some figures may appear in colour only in the online journal)

1. Introduction: theory and simulation in the nuclear fusion era

In developing a plan for the next EU Framework Programme for Research and Technological Development (2021–2027), *Horizon EUROPE*, European researchers are looking a decade into the future. Over that time, ground-breaking deuterium-tritium experiments will have been completed on JET; JT-60SA will be operating as a joint EU-Japan facility; ITER will have produced its first plasma and will be implementing the ITER research plan; the IFMIF-DONES facility (International Fusion Materials Irradiation Facility-DEMO Oriented NEutron Source), will be providing early data for materials to be used in the harsh conditions of a fusion power plant; Wendelstein 7-X will have assessed the performance of optimized stellarators in steady-state operation; the potential of spherical tokamaks for fusion power will become clearer, and, importantly, the design of the prototype fusion reactor (DEMO) in Europe will be significantly advanced (Federici *et al* 2019).

The step from ITER to DEMO is bold and challenging. Furthermore, DEMO goes beyond experiment—it is a *demonstration* of the technical potential of fusion energy, and therefore one has to design the infrastructure, components, control systems and plasma scenarios with a high degree of confidence. Given the extrapolation in conditions from ITER to DEMO, and from IFMIF-DONES to DEMO, the only way to achieve the required certainty in predictive capability is via rigorous, science-based models. High-fidelity theory-based plasma models for the integrated scenarios including plasma exhaust are needed in support of the experiments to bridge the gaps between present facilities and ITER and then DEMO.

With ITER and DEMO, the fusion programme enters the nuclear era where theory and simulation both in the engineering and physics domain will play an important role. Indeed, fusion facilities will have to address safety and nuclear licensing issues that require a deep knowledge of the operational domain and limits. Efficient, reliable and rapid tools for designing and prototyping a fusion power plant will be needed. It will also require efficient tools to master plasma operation in a safe and controlled manner. Systematic and accurate preparation of the experimental programme using numerical simulations with various levels of sophistication will be implemented in order to minimize the risk of purely empirical approaches. This will help to efficiently optimize the experimental time devoted to the development and achievement of sophisticated scenarios for the operation of nuclear facilities while optimizing the operating cost. This will require a mastery of the operation actuators, in order to ensure machine protection and safety via reliable control algorithms implemented in the plant and plasma control systems. In this context, theory

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[24] ITER ('The Way' in Latin) is the world's largest tokamak under construction in the south of France: a magnetic fusion device that has been designed to prove the feasibility of fusion as a large-scale and carbon-free source of energy (https://www.iter.org/).

and simulations both in the engineering and physics domains have the potential to accelerate the development of fusion energy.

Experimental data from ITER and IFMIF-DONES are essential, but not sufficient to design DEMO with confidence if we do not also have the tools available to predict plasma and materials performance, and integrate that knowledge into a modern computational approach to optimize plasma operation and engineering design. Therefore, it is timely to prepare this transition with a coordinated, comprehensive theory, simulation, verification and validation programme to maximize the benefit delivered from investment in large facilities. This aspect is recognized in the revised version of the Research Roadmap for the Realisation of Fusion Energy (Donné *et al* 2017, European Research Roadmap to the Realisation of Fusion Energy 2018) which states 'For all the missions, a theory and modelling effort integrated tightly with the experimental programme will be crucial in providing the capability of extrapolating the available results to ITER, DEMO and commercial fusion power plants through carefully validated models and codes'. An empirical approach will not be sufficient to bridge the gap between an experimental facility like ITER and a demonstration facility-like DEMO as stated in the EUROfusion[25] Research Roadmap 'It has become clear that a strong theory and modelling programme is essential because empirically-based predictions are uncertain in unexplored environments like ITER and particularly DEMO, and this will be a stronger focus than foreseen earlier. It will make use of advanced computational techniques and high performance computers.' Indeed, major advances in computational hardware and computer science are anticipated over the next decade and into the ITER era. This could be game-changing for those who are positioned to exploit it. The challenge is to develop a strategy that can evolve to maximize the benefits of the anticipated revolution in computational capability. This requires an integrated while flexible approach to modelling—an approach that brings together fusion physicists, materials scientists and engineers with a new generation of mathematicians and computer scientists within the same organisational framework.

The EUROfusion consortium has initiated a coordination in theory and advanced simulation to address some of the challenges of the fusion research in the next EU Framework Programme for Research and Technological Development (from 2021 through to 2027), *Horizon EUROPE.* This initiative is called E-TASC, which stands for EUROfusion-Theory and Advanced Simulation Coordination. This paper[26] will briefly describe the general and guiding principles of E-TASC without focusing on the detailed implementation aspects (section 2 of the paper). Then, in section 3, a high-level overview of the scientific results obtained in a pilot phase (2019–2020) of E-TASC will be briefly described, while highlighting the importance of further progress in computational methods and computer performance. Indeed, in 2019 and 2020, five theories and simulation tasks were initiated addressing some challenges of the Fusion Research Roadmap. In section 3 and in the conclusion part, long terms prospects of the E-TASC beyond 2020 will be provided.

2. General principles of E-TASC

In this context, with an increased emphasis on theory and simulation for preparing ITER operations, for exploiting the optimized Helical Axis Advanced Stellarator (HELIAS) line of research, and designing DEMO, it was concluded at the EUROfusion level that it is timely and important, to develop and implement a coherent programme of theory, simulation, verification and validation (TSVV). Fundamental research and development are key enablers that must be retained within the programme to advance our understanding of magnetic confinement facilities and to improve predictive capabilities. These advances will underpin the production of a high-quality suite of 'EUROfusion standard' software (building on the research software) to model data from EUROfusion facilities and to reliably extrapolate to future devices, thus informing ITER operation and the design of DEMO (including both tokamak and stellarator HELIAS versions). To deliver these outcomes, a higher level of EUROfusion coordination is required that will integrate fusion science and engineering with emerging advances in computing: this is the vision for the E-TASC initiative.

A rigorous scientific approach is essential to provide the necessary reliability in predictions. To achieve this, E-TASC will facilitate teams with an appropriate mix of theoreticians to develop models and test simulation output; experimentalists to design rigorous validation tests of the models; computational physicists/materials scientists and applied mathematicians to develop and implement optimized numerical methods, and computer scientists to ensure the code developments keep pace with the evolution of computer architecture, data management, algorithms and hardware.

Strength in analytic theory and computer modelling will develop world-class, verified codes, while the exploitation of experimental facilities will provide validation that is key to confident extrapolation. One role of E-TASC is to coordinate this activity to provide reliable and predictive 'EUROfusion-standard' fusion simulation tools. It is proposed that a new activity in computer science should be introduced in this effort to ensure that the EUROfusion simulation capability remains at the forefront, while hardware infrastructure, data management capabilities, and software techniques advance.

Different tools are needed on different timescales to progressively move towards the integrated design, construction and operation of DEMO and fusion reactors. The tools will be required to (a) prepare for JT-60SA; (b) address the science and technology challenges to optimize the path towards

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[25] EUROfusion is a consortium of European institutes and laboratories coordinating the fusion programme on behalf of the European Commission with the aim of delivering the fusion research roadmap. The goal of the fusion research roadmap is to deliver fusion electricity to the grid early in the second half of this century.

[26] The paper is a summary of the overview oral presentation given at the 1st Spanish Fusion HPC Workshop on 27 November 2020.

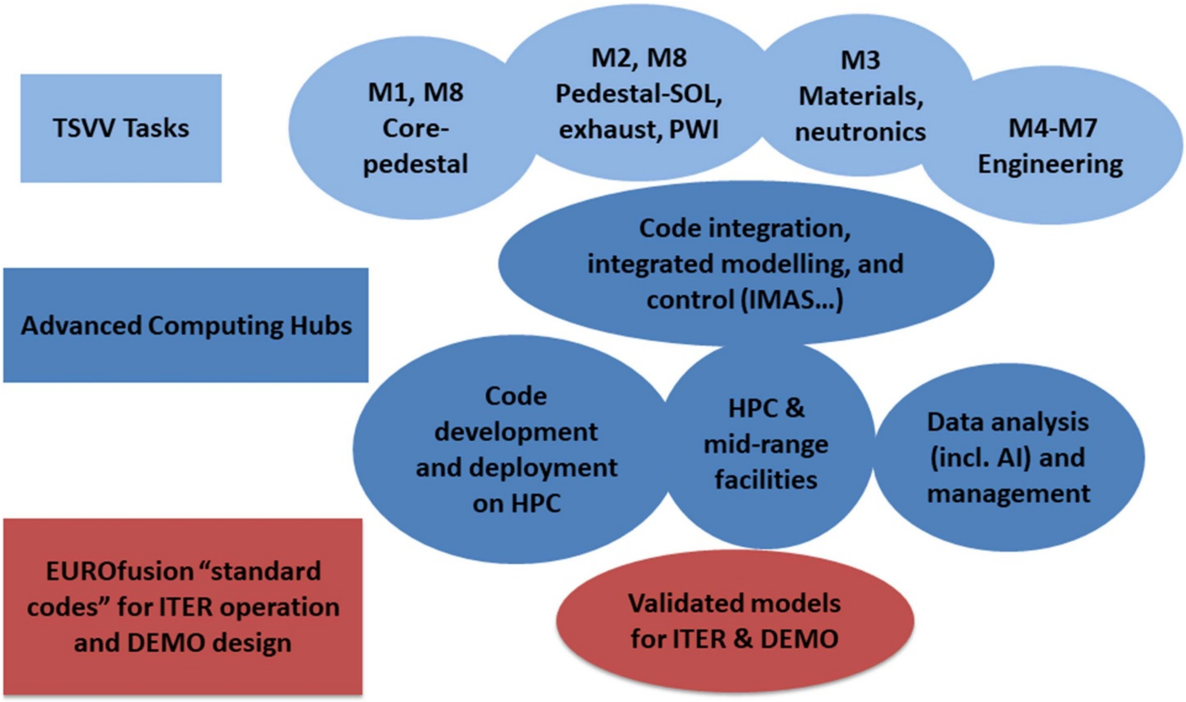

Figure 1. Sketch of the E-TASC programme in support of the EUROfusion Roadmap missions as a mix of coordinated de-centralized TSVV tasks and more centralized ACH efforts operating in a virtuous cycle to deliver validated models for ITER and DEMO. Each TSVV supports selected Missions (M1–M8) of the Research Roadmap for the Realisation of Fusion Energy (European Research Roadmap to the Realisation of Fusion Energy 2018). Mission 1 (M1): plasma regimes of operation; Mission 2 (M2): heat-exhaust systems; Mission 3 (M3): neutron tolerant materials; Mission 4 (M4): tritium self-sufficiency; Mission 5 (M5): implementation of the intrinsic safety features of fusion; Mission 6 (M6): integrated DEMO design and system development; Mission 7 (M7): competitive cost of electricity; Mission 8 (M8): stellarators.

ITER's goals; (c) predict and interpret the outputs from ITER operation; (d) predict, interpret and extrapolate properties of irradiated materials; (e) develop engineering design options for DEMO, (f) develop new digital approaches to engineering design, including integrated components and, potentially, a complete digital model for DEMO and (g) design the next-generation of optimized stellarators. This range of objectives requires a multi-fidelity approach, with the highest fidelity required to improve our fundamental science understanding and to develop more reliable 'reduced models' that can be used in lower fidelity modelling of the whole device (integrated modelling, plasma discharge simulator for pulse preparation) and in real-time applications. Ensuring sufficiently accurate models across all applications, or understanding their regimes of validity, will rely on the quality of scientific input from first principles-based simulations, which will in turn require advances in fundamental theory and computing.

A fundamental philosophy within E-TASC is that the best, most innovative theory and simulation research is performed when it is driven by the scientists and engineers themselves. Nevertheless, the production of EUROfusion standard software requires a coordinated, directed approach. To accommodate both, two inter-linked structures have been implemented (as illustrated in figure 1):

(a) Specific projects, called TSVV Tasks, accommodate fundamental research in science, engineering and technology addressing key questions of the fusion roadmap missions.

(b) Advanced computing hubs (ACHs) which provide the scientific computing, data management, code integration, and/or software engineering support for the TSVVs (and indeed the entire EUROfusion theory/simulation program) and help to develop a new portfolio of EUROfusion 'standard software' for the R&D programme in support of ITER, associated facilities and DEMO design.

2.1. TSVV tasks

The fundamental research will be performed via a set of TSVV Tasks which are driven by the fusion R&D community and address questions or issues within the eight missions of the Fusion Roadmap. Each task will be closely linked to ACHs so that they can (a) benefit from the expertise in these Hubs, and (b) feed science and engineering breakthroughs into the ACHs to inform the development of software following well defined 'EUROfusion-standard' (c.f. sub-section 2.3).

One of the objectives of the TSVV tasks is to provide validated predictive capabilities by turning existing research codes into professional and widely used tools and by developing new codes to fill some gaps. The scientific vision is generally expected to be based on a multi-fidelity approach (ranging from first-principles-based models to reduced models that can be used in whole device modelling and for real-time control applications), including specific plans for verification, validation, and uncertainty quantification (VVUQ). In addition, it is understood that all participants of a given TSVV task share up-to-date development versions of the source codes and use a common development platform following modern software engineering standards. The software products developed in this context (EUROfusion standard software) are to be designed to benefit a wide range of users across EUROfusion, well beyond the team of code developers, with free availability (within EUROfusion) of up-to-date release versions of the source codes to be used for production runs.

The main research areas (addressing both tokamak and stellarator applications) that should be pursued are

(a) Core and pedestal plasma physics;
(b) Pedestal, scrape-off layer (SOL) and divertor plasma physics and plasma-wall interaction;
(c) Materials and neutronics modelling;
(d) Engineering and reactor design.

It is important to note that the research areas are all closely coupled. The core plasma couples to the SOL and divertor via the pedestal; this complex plasma system couples to the materials via the divertor and wall, both directly and via radiation (and neutrons in ITER and DEMO), while the materials choices, the need to breed tritium and the divertor design (for example) influence the engineering design. While E-TASC will seek to make new physics, technology and engineering advances in each of the areas at relatively high fidelity and rigor, it should also support a parallel activity to develop a framework that ultimately, but progressively, works towards integration of all aspects towards whole devices modelling.

2.2. ACHs

A key element in the implementation of the E-TASC approach consists of setting up ACHs in several EUROfusion labs, involving fusion theorists, applied mathematicians, experts in high-performance computing, as well as experts in data science and intelligent systems. ACHs activities call for a more focused and centralized approach. The ACHs are expected to provide essential expertise and support in scientific computing and software engineering for the E-TASC initiative and for the entire EUROfusion Theory and Simulation Programme (plasma physics, fusion materials research, and fusion engineering) as highlighted in the EUROfusion roadmap. ACHs will also help develop a suitable portfolio of EUROfusion standard software for the European R&D programme in support of ITER, DEMO, HELIAS and associated facilities. This support should include advanced computational techniques for high-performance computing on emerging Exascale hardware. This programme will support a multi-fidelity approach that encompasses:

(a) large-scale first-principles modelling on high-end supercomputers (towards Exascale);
(b) intermediate-scale first-principles and integrated modelling on mid-range platforms;
(c) fast simulators, or reduced models, that can be used for whole device modelling on small computers and in systems codes;
(d) database management (e.g. simulation and multi-machine databases) and data visualisation.

Each ACH will be organized around a limited set of specific, fusion-relevant themes in computer science, scientific computing, data management, code integration, and software engineering. To cover the EUROfusion requirements, the support provided by the ACHs have been classified into three categories:

- Cat. 1—High Performance Computing: scalable algorithms, code parallelization and performance optimization, code refactoring, GPU-enabling, preparing codes for Exascale etc.
- Cat. 2—integrated modelling and control: code adaptation to the integrated modelling and analysis suite (IMAS) format to support both plasma operation and research activities on ITER, IMAS framework development, code integration etc.
- Cat. 3—data management: open access, data management, data analysis tools, aspects of artificial intelligence and VVUQ etc.

The IMAS system, based on a machine-generic data dictionary (Imbeaux *et al* 2015), is a key standardization tool for E-TASC and EUROfusion data and code integration. Indeed, it has proven to be an efficient platform for multi-facilities data analysis, verification and validation and for multi-codes integration. Various tools have been recently developed for the mapping of experimental data into IMAS interface data structure for the different EUROfusion tokamaks (Romanelli *et al* 2020) which will facilitate model validation and data analysis across different facilities. Finally, to enable the large scale numerical simulations essential for the programme, EUROfusion will continue to support a dedicated High Performance Computing platform. This includes support for the centralized integrated modelling computing platform—the so-called Gateway.

The expertise and skill sets differ for the TSVV Tasks and the ACHs. For the TSVV Tasks, the teams will come largely from the fusion community, and be a mix of theoretical, experimental and computational scientists and engineers; this is where the frontier, community-led fusion science and technology is performed. ACHs may require some fusion-specific expertise, but will largely be formed of software engineers and computer scientists; this expertise will apply frontier computer science to fusion problems and our EUROfusion-standard software.

2.3. EUROfusion-standard software

Within E-TASC, two types of software are distinguished. On the one hand, the ‘research software’ is typically developed within the TSVV tasks or in the broader community. It tends to aim at addressing specific scientific or engineering questions and has a user base that often does not extend much beyond the code development team (although there are exceptions). The majority of the current EUROfusion software falls in this category, and while this will continue to play an important role in the future, it is clear that several significant challenges ahead—like supporting or even guiding ITER operation and DEMO design—call for a more systematic approach. Consequently, E-TASC will provide the platform and support to develop the so-called EUROfusion-standard software, taking the development, dissemination, and exploitation of fusion software to a new level.

EUROfusion-standard softwares will be developed by applying a very rigorous and consistent quality assurance process across all E-TASC activities; it will be 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 (continuous integration, 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 etc);
- specific plans for code verification and validation 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.

The development of EUROfusion standard softwares is to be primarily executed by the ACHs, using tight feedback loops involving the main code authors including physicists and engineers in the TSVV Tasks. In some cases, this software is to be developed from scratch, while in many instances the new codes will be developed and refactored from existing codes to become part of the EUROfusion-standard software suite.

3. Overview of the results from the E-TASC pilot phase (2019–2020)

Before deploying and implementing the full E-TASC infrastructure and programme within Horizon Europe (2021–2027), it was decided to have a two year's pilot phase involving five pilot tasks operating under the 2019–2020 *Horizon 2020* programme. The adopted pilot tasks had their main foci on fusion science activities relating to fusion roadmap missions M1 (plasma regimes of operation), M2 (heat-exhaust systems activities), and M8 (stellarators). In this initial phase without the implementation of the ACHs structure, the five TSVV tasks relied on the existing High Level Support Team and the access to dedicated CPU time on the MARCONI-Fusion supercomputer. MARCONI-Fusion is operated by CINECA (Bologna, Italy) with ten Peta-Flops peak dedicated to EUROfusion in its present phase (2019–2023). A small range platform (the so-called EUROfusion Gateway) for development, testing and distribution of codes and data for integrated modelling was made available on MARCONI-Fusion as well but with a specifically dedicated infrastructure.

The five pilot TSVV tasks briefly reviewed within this section are as follow:

(a) Towards a validated predictive capability of the low to high (L-H) transition and pedestal physics;
(b) Electron runaway in tokamak disruptions in the presence of massive material injection (MMI);
(c) Fast code for the calculation of neoclassical toroidal viscosity (NTV) in stellarators and tokamaks;
(d) Development of a neutral gas kinetics modular code;
(e) European edge and boundary code for reactor relevant devices.

3.1. Towards a validated predictive capability of the L-H transition and pedestal physics

This TSVV task addresses one of the grand challenges of fusion research: the ability to predict the transition from L-H confinement regime and its various characteristics. The long-term goal is to develop a validated predictive capability of the L-H transition including pedestal physics and the mitigation or avoidance of edge localized modes in the context of a multi-fidelity approach, from gyrokinetic (GK) to reduced models for ultimately real-time application.

In the first phase (2019–20) of the project, the focus was on using GK simulation and theory (e.g. Jenko *et al* 2005, Brizard and Hahm 2007, Falchetto *et al* 2008, Garbet 2010, Krommes 2012) to characterize the L-mode edge and H-mode pedestal just before and after the L-H transition and on investigating the sources and dynamics of the radial electric field leading to an improved confinement regime. The task is exploiting the state-of-the-art in GK simulation of the tokamak edge, developing reduced models, while addressing key aspects of Verification, Validation, and Uncertainty, Quantification. As summarized in figure 2, the overall project structure is sub-divided in five main pillars leading to an overall vision for integration beyond 2021:

(a) GK advancements for tokamak edge;
(b) L-mode characterization prior to L-H-transition;
(c) Study H-mode pedestal after L-H transition;
(d) Investigate the plasma radial electric field (E_r) sources & dynamics;
(e) Address key aspects of VVUQ.

All the activities performed within this broad task cannot be reviewed here, but two typical examples of the work performed are provided below: (a) on the investigation of the radial electric field dynamics, and, (b) on the validation aspects on JET.

In the first example, it has been shown in GK simulations with the GYSELA code (Grandgirard *et al* 2016) that a radial electric field well develops in simulations performed with an axi-symmetric limiter by comparing cases with and without

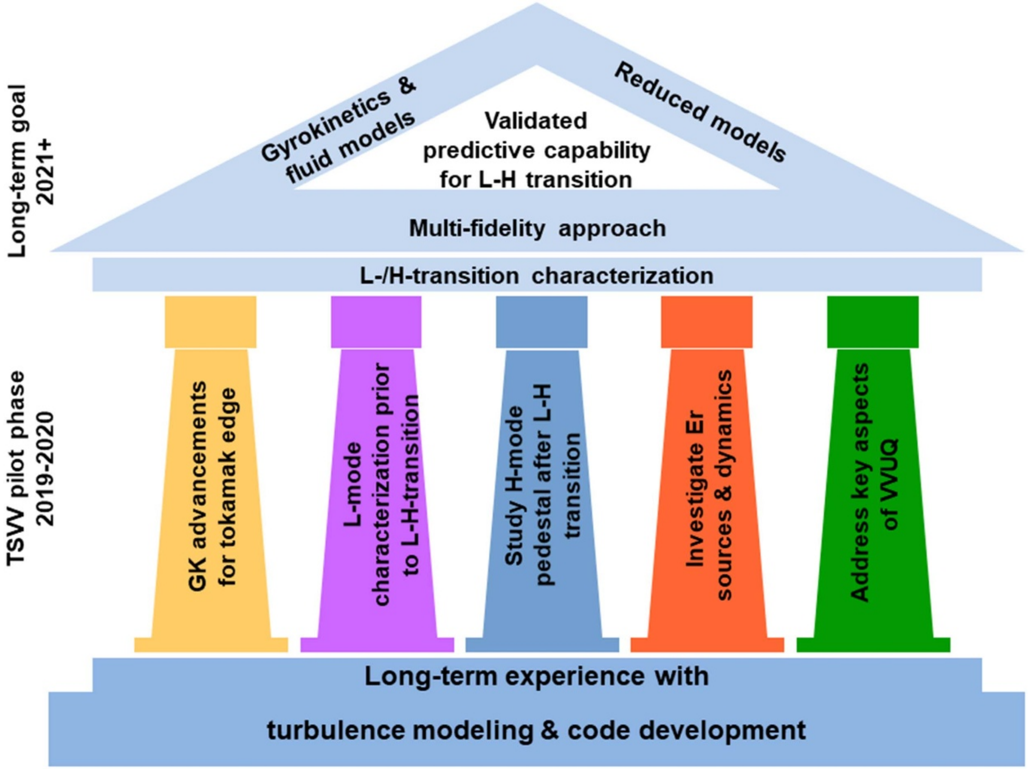

Figure 2. Overview of the project structure and the key pillars of the activity (Görler 2021).

limiter (Dif-Pradalier *et al* 2020). GYSELA models the ions and trapped electrons gyro-kinetically in the core and edge regions as well as the closed/open field line transition and the SOL through the introduction of a simplified limiter mimicking the role of a heat and momentum sink. A spontaneous radially-localized shear layer develops at the transition from closed to open field lines only with the limiter and with an interface to the SOL. The shear in the radial electric field is associated with the mild steepening of the pressure profile. The spontaneous emergence of a stable and localized transport barrier at the transition between closed and open field lines, is interpreted as a possible prelude to the formation of a pedestal in the first principles simulations as in tokamaks experiments.

The second example is the more systematic exploitation of GK simulations to interpret the structure of the Joint European Torus (JET)[27] plasma pressure pedestals with the ITER Like Wall (ILW, tungsten divertor and beryllium chamber, reference e.g. Pamela *et al* 2007, Matthews *et al* 2011) for different levels of applied power and injected neutral gas at the plasma boundary. Indeed, ITER-baseline plasmas at JET-ILW have been limited to lower pedestal electron temperatures compared to their JET-C (carbon-wall) counterparts (e.g. Frassinetti *et al* 2019). As a consequence, more heating power to achieve good pedestal performance is required with the ILW compared to C-wall. In addition, high fuelling is required with the JET-ILW to mitigate the W accumulation effect that further degrades the pedestal. Understanding the fundamental structure of the JET pedestal with a metallic wall is essential for extrapolating the results towards ITER with a similar selection of wall materials (Hatch *et al* 2019). In this context, the local GK calculations with the gyrokinetic plasma turbulence code GENE (Gyrokinetic Electromagnetic Numerical Experiment) (Jenko *et al* 2000) have been performed from a series of JET-ILW type I ELMy H-modes discharges operating with similar experimental inputs but at different levels of power and gas fuelling (Chapman *et al* 2021). It has been shown that the dominant slab-electron temperature gradient (ETG) driven modes (with high $k_{//}$) combined with neoclassical ion heat transport can account for the transport power loss across the pedestal when this can be measured in several of these JET discharges.

3.2. Runaway electrons in tokamak disruptions in the presence of MMI

Understanding the processes governing runaway electrons (RE) generation during MMI is crucial for interpreting existing disruption mitigation experiments and for the design of an effective disruption mitigation system in ITER, where RE currents of several Mega-Amperes can severely damage the plasma-facing components. The long-term objective of this TSVV task is to develop

(a) a comprehensive theoretical-numerical model framework to reliably predict RE dynamics in disruptions with non-equilibrium atomic physics for medium size tokamaks, JET, JT60-SA and ITER;

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[27] Joint European Torus (https://www.euro-fusion.org/devices/jet/, https://ccfe.ukaea.uk/research/joint-european-torus/).

(b) a model of RE mitigation by MMI and suggestions for improving RE mitigation scheme;
(c) a framework for the validation process against experimental data by developing synthetic radiation diagnostic tools.

Integrated simulation of RE requires computationally expensive kinetic models that are self-consistently coupled to the evolution of the background plasma parameters. The computational expense has been reduced by using parameterized RE generation rates rather than solving the full kinetic problem, Hesslow and co-workers (Hesslow *et al* 2019a; 2019b) have developed an improved and reduced model for the Dreicer generation rate for a wide range of plasma parameters and impurities. The need to include screening effects in partially ionized plasmas is important to simulate disruption mitigation scenarios with MMI to mitigate the disruption effects. For this purpose, a multilayer neural network has been trained on data obtained from kinetic simulations to accurately estimate the runaway generation rate. By implementing it in a fluid RE modelling tool(s), it has been shown that the improved generation rates lead to significant differences in the self-consistent runaway dynamics as compared to the results using the previously available formulas for the runaway generation rate. Numerical solutions of the coupled equations of runaway generation and electric-field diffusion (e.g. GO model by Smith *et al* 2006) in a JET-like disruptive scenario has shown that the plateau runaway current was significantly reduced when using the runaway generation rate by the neural network instead of the Connor–Hastie formula (Connor and Hastie 1975). The results demonstrate the need to account for partially ionized atoms for realistic modelling of Dreicer generation.

In this context, integrated transport simulations of the plasma disruption (induced by massive gas injection) up to the established RE beam have been performed and validated in an ASDEX Upgrade experiment (Linder *et al* 2020). A fluid approach has been used for calculating the evolution of the plasma background (with the ASTRA code (Fable *et al* 2013)), the impurities (with the STRAHL code (Dux *et al* 1999)) and the runaway electrons beam where the RE growth and decay physics processes have been captured in presence of partially ionized high-Z impurities (with REGIA for RE Generation In Astra (Linder *et al* 2020)). It was found that the generation of REs in the ASDEX Upgrade discharge #33108 is described reasonably well within the fluid simulation (Linder *et al* 2020) by reproducing the final RE current obtained experimentally when the impact of partially ionized impurities on RE generation are included through application of the models by Hesslow *et al* (2019a), Hesslow *et al* (2019b). Hence, the simulations reproduce reasonably well both the evolution of the RE current and Hard x-ray measurements. Finally, it was noted that the model will have to be updated for the simulation of the JET or ITER Deuterium-Tritium experiments to also include RE generation mechanisms due to nuclear processes (e.g. tritium decay, Compton scattering).

Synthetic radiation diagnostic tools are essential for an accurate validation of the RE simulation against experimental measurements. The synchrotron radiation emission of the relativistic RE is measured in order to diagnose characteristics of the RE distribution function. Synthetic synchrotron radiation diagnostics have been developed to be compared directly to experimental data. Analyses of visible-light camera images of the synchrotron emission from RE have been performed for the ASDEX Upgrade discharge #35628 (Hoppe *et al* 2021) as shown in figure 3. In the forward modelling (solution of a fluid-kinetic equation system) the electron kinetic code CODE (Landreman *et al* 2014, Stahl *et al* 2016) and the fluid code Go (Smith *et al* 2006, Fehér *et al* 2011, Papp *et al* 2013) have been coupled. This approach allows to self-consistently solve Faraday's law for the electric-field evolution together with the rate equations for the evolution of the temperature and ion charge states in the presence of cold argon impurities. This coupled kinetic-fluid framework permits the simulation of the evolution of the runaway electrons distribution function (radius, energy, pitch) during the current-quench and runaway plateau phases of the disruption, with a prescribed runaway seed profile which is assumed to have survived the thermal quench. The simulations reveal that the evolution of the runaway distribution is well-described by a two-component process: an initial hot tail seed population, which is accelerated to energies ranging between 25 and 50 MeV during the current quench, together with an avalanche runaway tail which has an exponentially decreasing energy spectrum. During the runaway plateau, the evolution of the runaway distribution is found to mainly consist of pitch-angle relaxation. It has been concluded that, although the avalanche component carries the vast majority of the current, it is the high-energy seed-remnant that dominates the synchrotron emission.

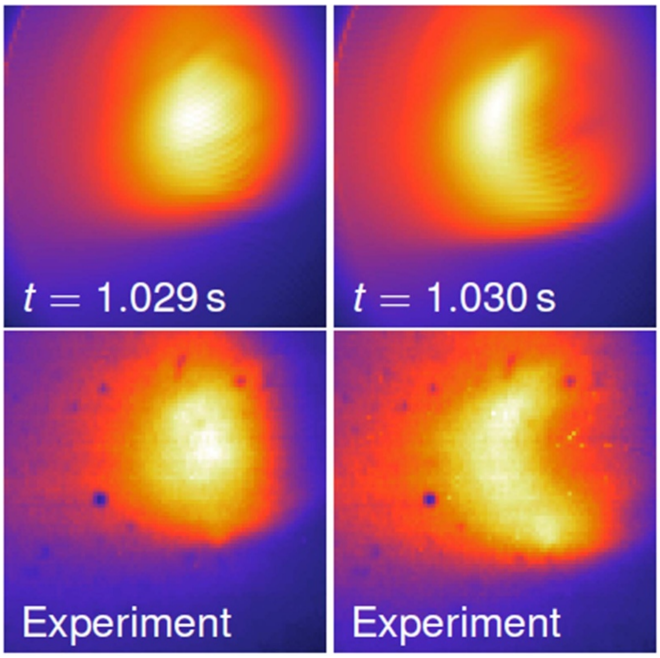

Figure 3. Runaway electrons radial distribution reconstruction [ASDEX Upgrade discharge #35628]. Synthetic (upper) and measured (lower) synchrotron images at $t = 1.029$ s and $t = 1.030$ s. Reproduced from Hoppe *et al* (2021). CC BY 4.0.

3.3. Fast code for the calculation of neoclassical toroidal viscosity in stellarators and tokamaks

This specific and well-focused TSVV task is addressing in a synergetic manner activities for both stellarators and tokamaks configurations (Velasco *et al* 2020). Indeed, numerical tools developed for three-dimensional, 3D, magnetic stellarator configurations can be adapted for solving specific aspects of tokamak physics. For instance, an accurate calculation of radial neoclassical transport is important for both tokamaks and stellarators. Intrinsically, 3D magnetic configurations of stellarators lead to specific neoclassical transport regimes that produce radial energy transport comparable, and often larger, than the turbulent fluxes. In tokamaks, deviation from axisymmetry can result in a significant neoclassical damping of the toroidal rotation and change the confinement properties of the tokamak configuration. A fast code for the calculation of the toroidal neoclassical viscosity in present and future tokamaks such as ITER has therefore been developed by adapting numerical tools developed for stellarators to tokamaks with broken toroidal symmetry (e.g. toroidal magnetic ripple or resonant magnetic perturbations).

Recent results include the derivation of the equations that allow a fast and accurate computation of the radial neoclassical transport in low collisionality regimes, and the development of numerical tools to solve such equations. KNOSOS (Velasco *et al* 2021) is a freely-available (Velasco 2022) open-source code that provides a fast computation of low collisionality neoclassical transport in 3D magnetic confinement devices by rigorously solving the radially local bounce-averaged drift kinetic equation coupled to the quasi-neutrality equation. KNOSOS incorporates physics ingredients often neglected in local 3D neoclassical simulations, such as the components of the magnetic drift and the electric field that are tangent to magnetic surfaces, as well as the effect of the local magnetic shear. It has been shown that, by characterizing plasmas of several devices, KNOSOS reproduces (where applicable) the results of standard neoclassical codes while being typically two orders of magnitude faster. In addition, KNOSOS describes the superbanana-plateau transport regime of stellarators and non-axisymmetric tokamaks by retaining the effect of the component of the magnetic drift that is tangent to magnetic surfaces. Therefore, KNOSOS provides the calculation of the NTV in tokamaks with broken axi-symmetry configurations at low value of plasma collisionality. Several applications of KNOSOS are planned for stellarators and tokamaks, including detailed validation activities against experimental data for Wendelstein 7-X, LHD and ASDEX Upgrade. As a preliminary application, a comparison of the electron NTV calculated with NEO-2 (Kernbichler *et al* 2016) and KNOSOS for one ASDEX Upgrade discharge is illustrated in figure 4. The preliminary results indicate a good agreement between the two codes outside mid-radius with a computing time ∼10 s per flux-surface. It should be pointed out that activity is ongoing to understand the difference between the two codes for tokamak geometry, and, to ultimately improve the calculation inside the normalized plasma radius of 0.5.

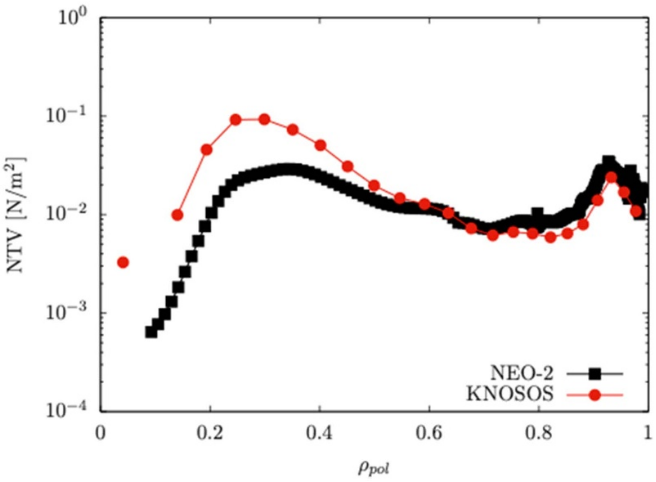

Figure 4. Electron NTV calculated with NEO-2 (Black line-Squares) and KNOSOS (Red line—circles) codes for ASDEX Upgrade discharge #30835 (NEO-2 simulations from Martitsch *et al* 2016).

3.4. Development of a neutral gas kinetics modular code

Neutral gas physics and neutral interactions with the plasma background are key aspects for describing the plasma edge and divertor physics in present and future tokamak or stellarator facilities. Indeed, predictions of ITER and future fusion reactor plasma edge and plasma-wall interaction behaviour rely on the modelling of the detachment phenomenon which are essential for solving the power exhaust challenges of the mission 2 of the fusion roadmap (c.f. also next subsection 3.5).

The EIRENE 3D Monte-Carlo code (Reiter *et al* 2005) is used worldwide to model neutral transport in tokamaks (e.g. Medium Size Tokamaks, EAST, JET, JT60-U, JT-60SA, ITER) with and without magnetic perturbations, stellarators and helical devices (e.g. TJ-II, LHD, W7-X). EIRENE is coupled in different code packages such as SOLPS-ITER (Wiesen *et al* 2015) and SOLEDGE2D-EIRENE (Bufferand *et al* 2015). The objective of this recently initiated TSVV task is to improve the accuracy and performance of various approaches within EIRENE to simulate the neutral gas dynamics for practical applications to ITER and fusion reactor. It should be noted that modelling of transients which require time-dependent simulations poses additional challenges for the code performance. Moreover, including the louvre areas and pump ducts into the simulation volume was proven to be significant for the pumping speed and penetration of neutrals modelling including molecules into the plasma with isotopic effects. An accurate prediction of heat and particle fluxes outside the divertor plates also necessitate an extended grid allowing the far-SOL flows to be included into the modelling (Dekeyser *et al* 2021).

The Monte-Carlo approach performs well in cases where neutrals can be treated as kinetic particles with large mean-free paths between collisions. However, the neutral collisionality will increase dramatically in high-density regions leading to

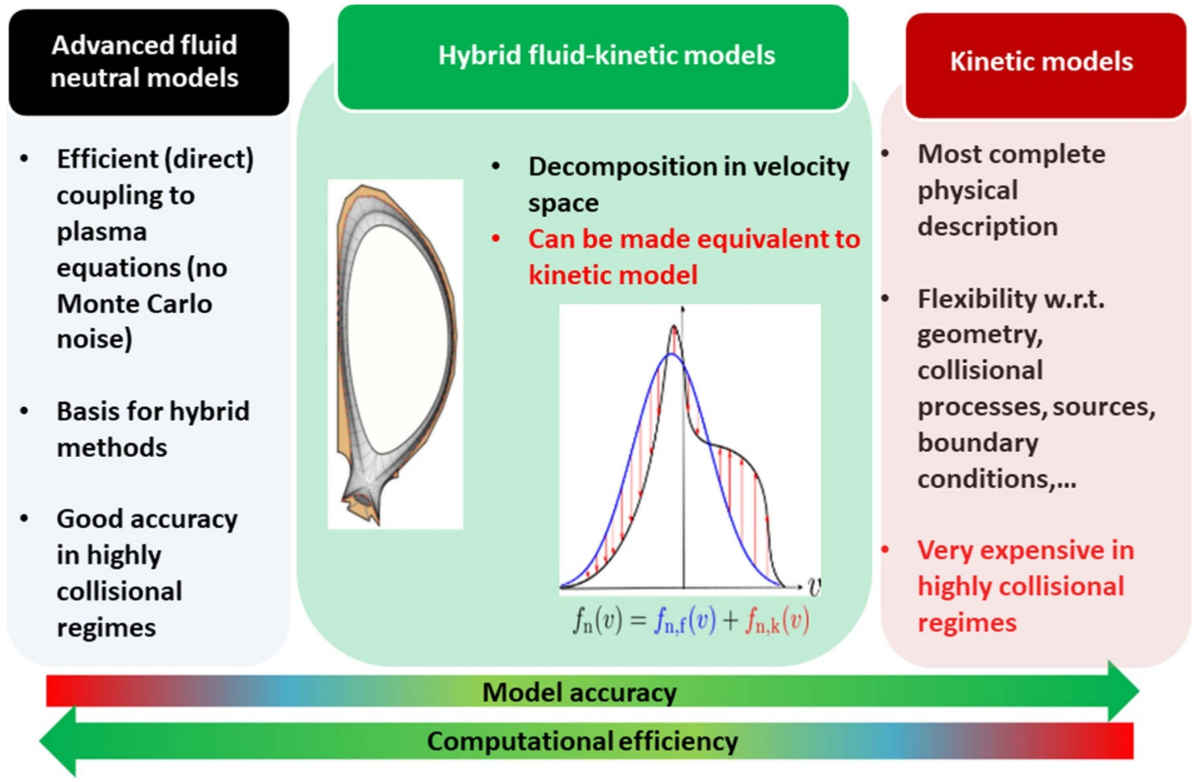

Figure 5. Overview of the hierarchy of the neutral gas dynamics model (Borodin *et al* 2021).

much more complex trajectories with simulations of competing atomic and molecular reaction chains processes. This requires an increase of the codes performance by several orders of magnitude. Part of the effort may consist of 'brute force' acceleration of codes by refactoring and parallelization schemes. However, this will probably not be sufficient for computationally challenging simulations in high-collisional edge regions as anticipated for ITER, DEMO and fusion reactors. Fortunately, for these application domains, it is possible to treat a fraction of neutrals in a fluid approximation which is computationally efficient. It is worth noting that this approximation, known as advanced fluid neutral (AFN) approach, has been significantly improved (Horsten *et al* 2017). It is important to derive a hierarchy of models suitable for regions with various collisionalities and other relevant parameters ranging from pure kinetic (most accurate) to the fluid approach for performance. An illustration of the overview of the hierarchy of models for the different simulation approaches of the neutral gas dynamics is shown in a schematic diagram (c.f. figure 5). The overview of these methods including their relation and advantages is given in (Borodin *et al* 2021). The diagram graphically illustrates the trade-off that needs to be found between the model accuracy (fully kinetic model) and the computational efficiency (fluid model). In this context, hybrid fluid-kinetic models could provide an optimum between accuracy and computational efficiency for simulating ITER and DEMO. The intermediate hybrid approaches combine the advantages of both. For instance the so-called micro-macro hybrid (mMH) approach based on using a fraction of simulations done kinetically as a sort of correction term is seamless in the volume and theoretically fully equivalent to the full kinetic approach by the accuracy. The so-called spatial approach based on segregation of AFN and kinetic domains in space is a trade-off between accuracy and performance.

It has already been shown that hybrid fluid-kinetic approaches developed for the computational fluid dynamics-EIRENE packages combine acceptable computing performance with model accuracy approaching full kinetic simulations as shown in figure 6 with results obtained with the so-called mMH method in a slab geometry approximation.

Currently, the efforts are focused on the

(a) Fundamental and basic development of the hybrid approaches;
(b) Comparison against full-kinetic simulations to determine the gain in computational speed-up and optimal parameters;
(c) Assessment of the hybrid approach and their suitability for modelling new physics and operating domains at high edge collisionality in ITER or DEMO;
(d) Unification of the methods allowing e.g. combined mMH and spatially hybrid (SpH) simulations;
(e) Error assessment including particular contributions (bias, cancelation and statistical noise).

The OpenMP-MPI code parallelization and optimisation of the modelling atomic and molecular processes should progress in parallel. However, it should be stressed that the optimization

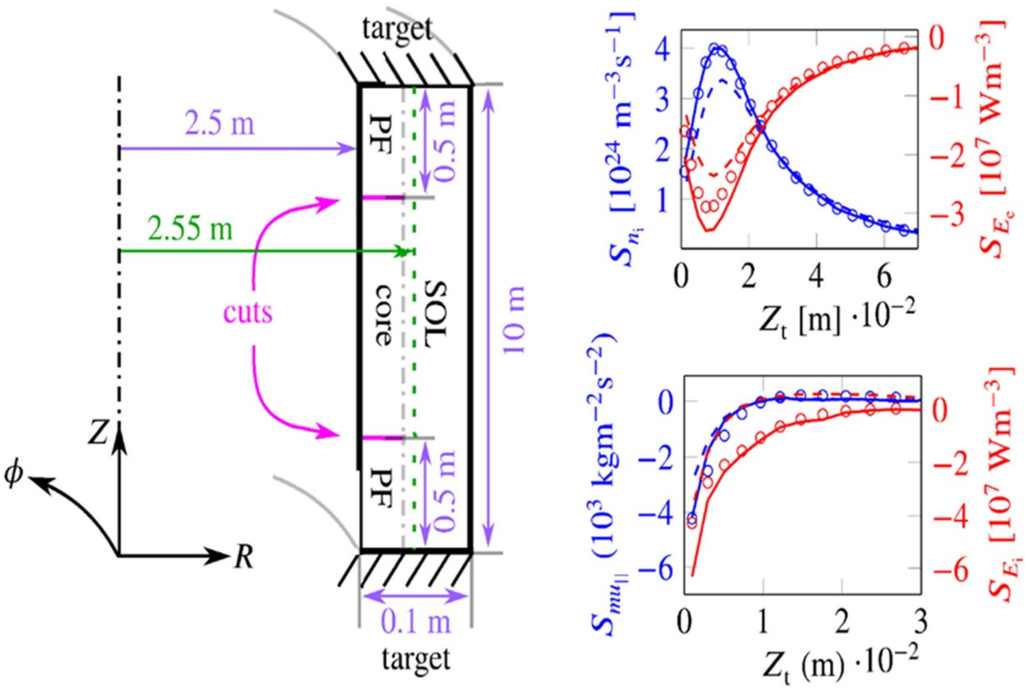

Figure 6. (Left) Poloidal cross section of the slab geometry with the different regions: core, private flux (PF) and scrape-off layer. (Right) results of the calculations performed using the pure kinetic, pure fluid, and hybrid fluid-kinetic models in slab geometry with JET-relevant parameters in high recycling conditions. Particle (S_{ni}), parallel momentum ($S_{\mathrm{mu}\|}$), ion energy sources (S_{Ei}) and electron energy sources (S_{Ee}) estimated along the selected flux tubes at major radius of 2.55 m with kinetic (solid lines), fluid (dashed line) and micro-macro fluid-kinetic hybridisation mMH (circles). Reproduced with permission from Horsten *et al* (2020). John Wiley & Sons. © 2020 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

procedure may depend on the final selection of the hybrid fluid-kinetic scheme.

The aim is to develop a neutral gas code (EIRENE) that provides a hierarchy of neutral (and trace ion) models with guidelines and automatic tools for hybridisation and parallelisation parameter optimisation to allow the end user to decide on an appropriate level of accuracy and performance depending on the problem to solve.

3.5. European edge and boundary code for reactor relevant devices

It is widely acknowledged that in the extreme conditions (in terms of exhaust and neutron fluxes) of a reactor relevant machine, handling the plasma exhaust towards the material surfaces of the device is of crucial importance, i.e. the so-called Mission 2 (Heat-Exhaust systems) of the 2012 and 2018 fusion roadmap (Fusion Electricity—A roadmap to the realisation of fusion energy 2012 and European Research Roadmap to the Realisation of Fusion Energy 2018). To extrapolate present day results to ITER and DEMO with sufficient confidence, adequate predictive capabilities, based on first principles insight, should be obtained through the development of both theoretical models for the plasma edge and innovative numerical codes applicable to the new generation of High Performance Computer (HPC). An effort in this direction must take into account the challenges of the particular operation conditions for DEMO and future fusion reactors, which are not encountered in current experiments and therefore even less often properly modelled.

High performance computing is evolving at a fast pace towards Exascale capabilities, which will allow unprecedented performance for scientific codes and these advances must be intercepted by the fusion community building on the existing effort. This challenging TSVV task is aimed at producing an agile software framework for ultimately developing a European edge and boundary code that builds on past experience and existing codes, and adopts a multi-fidelity approach that is able to exploit computational advances and perform simulations in conditions more relevant to ITER and DEMO. The task has included requirements analysis, software architecture and high-level design of the main modules with an overall picture of their interaction, identification of optimal algorithms, and creation of modular applications to test the scalability of the proposed solutions. This is to ensure predictive capability for heat and particle exhaust up to reactor relevant conditions by following a multi-fidelity approach with a hierarchy of models allowing users to optimize fidelity versus the computing time depending on the application. For large and high fidelity cases the codes(s) should be designed to run on Exascale HPC architectures with an objective of typically one month duration simulations for the most advanced first-principle simulations. The long-term scope of the task is to simulate the coupled plasma and neutral particles physics (c.f. section 3.4) in the SOL and in the region inside the separatrix in realistic 3D geometry with self-consistent cross-field turbulent transport.

In the initial phase of the project performed in 2019 and 2020, only part of the full programme has been realized and the initial focus has been on the definition of the physics basis and on the specification of the high-level design leading to the development of a reduced number of core modules of the code to test its potential capabilities and scalability. In this initial period, particular attention has been devoted to transfer any original concept to the suite of existing European edge codes, with the aim of maintaining their unique features during the period of development of the European edge and boundary code. The key challenges and initial results for this ambitious task are summarized below:

(a) Developing plasma models compatible with reactor conditions: for instance, the simulations should deal with four decades of collisionality range from the divertor to the pedestal which is beyond the domain of applicability of standard fluid models. Indeed, the applicability of Braginskii-like fluid models is questionable to describe the whole boundary region. In the context of the task, the recent development of the gyro-moment approach to the GK model has provided an ideal framework for the development of a multi-fidelity scheme to simulate the turbulent plasma dynamics in the boundary region of tokamak devices where collisions play an important role and cannot be ignored (Frei *et al* 2020 &, 2021, Bufferand *et al* 2021). Also, a new model of the high collisional plasma sheath has been developed (Tskhakaya 2021).
(b) Integrating the reactor relevant physics: additional physics is required in turbulence models for describing consistently the environment (neutrals, impurities…) (Tamain *et al* 2021, Bufferand *et al* 2022).
(c) Optimizing the codes for HPC application: during the pilot phase in 2019–2020, the focus was on optimization of common bottleneck of existing codes, i.e. the elliptic solvers for plasma potentials.
(d) Optimising algorithms and computational needs: assess and implement the advanced parallel discretization methods based on the flux coordinate independent approach (Hariri and Ottaviani 2013, Stegmeir *et al* 2016) for the reduction of computational needs. During the pilot phase in 2019–2020, the Hybrid Discontinuous Galerkin approach has been investigated.

Finally, it should be stressed that the ongoing development in computers performance and efficiency will be critical for the success of this challenging task. Indeed, for simulating the full 3D turbulence including the neutral and impurity physics in the SOL in proper realistic magnetic geometry of DEMO, the number of degrees of freedom (DOF) is typically two orders of magnitude higher compared to some of the largest computational fluid dynamics simulation as for instance the Peloton Project ($\sim$2 billion of DOF) (Blocken *et al* 2018). Indeed, Tamain (2021) has estimated that the DOF is around 200 billion for solving the heat and particle exhaust up to the reactor relevant conditions and size. Therefore, the challenge of the simulation of the edge and boundary for reactor relevant devices could only be addressed by following a holistic approach combining advances in HPC, optimization of the algorithms and computational methods suited for HPC and improvement in the integration of the most advanced physics.

4. Conclusion and prospects

A theory and advanced simulation programme, that is ‘essential because empirically based predictions are uncertain in unexplored environments like ITER and particularly DEMO’, has found a coordinating structure to support the full implementation of the fusion roadmap with the E-TASC proposal. Indeed, theory and advanced simulation can contribute to the development of optimized operational scenarios, help ensure machine protection, and, has the potential to accelerate the development of fusion energy. Via a synergy between TSVV tasks and ACHs, E-TASC will develop validated predictive capabilities for key challenges in fusion research for ITER and DEMO. An initial pilot phase was undertaken in 2019 and 2020 with five TSVV projects benefiting from the existing High Level Support Team and the access to a dedicated part of the MARCONI supercomputer (MARCONI-Fusion).

Following the initial phase in 2019–2020, it was decided in the context of the next EU framework programme, *Horizon Europe*, to initiate 14 TSVV projects for 2021–2025 (with progress to be reviewed by 2023) supported by five ACHs located in various EU laboratories. The ACHs are located as follows depending on the category to which they belong to:

- three ACHs have been selected to support activities on ‘High Performance Computing’ (Cat. 1) and are hosted respectively by
  - Germany (at the Max-Planck-Institut für Plasmaphysik (IPP), Garching);
  - Spain (at the Barcelona Supercomputing Center, Barcelona);
  - Switzerland (at the Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne).
- one ACH has been selected to support activities on ‘Integrated Modelling and Control’ (Cat. 2) located in Poland (at the Poznan Supercomputing and Networking Centre, IBCh Polish Academy of Sciences, Poznan);
- one ACH has been selected to support activities on ‘Data management’ (Cat. 3) located in Finland (at the University of Helsinki, Kumpula Campus, Helsinki).

The 14 TSVV tasks will address the following topics:

(a) Dynamics of RE in Tokamak Disruptions
(b) Impurity Sources, Transport, and Screening
(c) Integrated Modelling of Transient MHD Events
(d) Multi-Fidelity Systems Code for DEMO
(e) Neutral Gas Dynamics in the Edge
(f) Physics of Burning Plasmas
(g) Physics of the L-H Transition and Pedestals

(h) Physics Properties of Strongly Shaped Configurations
(i) Plasma Particle/Heat Exhaust: Fluid/Gyrofluid Edge Codes
(j) Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes
(k) Plasma-Wall Interaction in DEMO
(l) Stellarator Optimization
(m) Stellarator Turbulence Simulation
(n) Validated Frameworks for the Reliable Prediction of Plasma Performance and Operational Limits in Tokamaks

Progress will rely on (and should adapt to) advances in computing resources that will become available for large-scale simulation and integrated modelling. In this context, EUROfusion should continue its strategy of investment in computer resources based on large- and medium-size systems dedicated to fusion research, while the most extreme simulations requiring Exascale computation may be more effectively resourced through the EuroHPC initiative (EuroHPC Joint Undertaking 2021).

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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