Proposal for participation in a “Theory, Simulation, Validation and Verification” (TSVV) Task (*personal participant’s information removed*)

Title (c.f. Annex-2)	***TSVV Task 10: Physics of Burning Plasmas***
TSVV Task leader (name/e-mail)	***Oleksiy Mishchenko / alexey.mishchenko@ipp.mpg.de***
Lead beneficiary	MPG (Germany)
Project duration	**2021-2025 (-2027) : 5 years (7 years)**

TSVV Task leader

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Detailed workplan with timeline, milestones, SMART deliverables, and risk assessment (up to 10 pages)

Physics of burning plasmas in ITER or in a future DEMO reactor (tokamak and stellarator) is strongly affected by the presence of fusion-born alpha particles. Understanding of burning plasma physics requires a substantial theory and modelling effort, since present devices cannot generate alpha particles at the rate comparable to burning plasmas. Dynamics of burning plasmas is a multi-spatiotemporal-scale process where the energetic particles play a role of a mediator for the cross-scale couplings. In our project, we will develop dedicated tools and apply them to understand complex nonlinear dynamics of burning plasmas in both tokamak and stellarator geometries. Fast-particle physics, its coupling to the micro-turbulence and to the transport process will be considered, as well as MHD stability in presence of a large population of energetic particles, in accordance with the high-level deliverables.
The present proposal builds on and will expand the results and knowledge of three former Enabling Research (ENR) projects: “Theory and simulation of energetic particle dynamics and ensuing collective behaviors in fusion plasmas” (NLED), “Nonlinear interaction of Alfvénic and turbulent fluctuations in burning plasmas” (NAT), and “Multi-scale Energetic particle Transport in fusion devices” (MET). In our proposed TSVV project, we will develop the high-fidelity fully-gyrokinetic framework based on the existing codes ORB5 (tokamak geometry) and EUTERPE (stellarator geometry). These global gyrokinetic particle-in-cell codes will be refactored aiming at providing a common framework for simulations of electromagnetic

microturbulence coupled to energetic particles, and global modes (Alfvén Eigenmodes, Energetic Particle Modes, and MHD-type modes such as the internal kink instability) in burning plasmas. The unified ORB5&EUTERPE will generate high-fidelity simulation data both in tokamak and stellarator geometries. Reduced models for the energetic-particle dynamics developed within the proposed TSVV project or provided by the community will lead to much cheaper lower-fidelity simulation data. A combination of these complementary approaches, reduced models and the fully-gyrokinetic simulations developed by the proposed TSVV, will give a multi-fidelity description of the fast-particle dynamics for transport codes, such as the European Transport Simulator. For this integration, we will have a dedicated expert on integrated transport modelling in the proposed TSVV project. We will use the multi-fidelity description of the energetic-particle dynamics also to predict the MHD stability in presence of a significant fast-particle population. For this task, experts in MHD modelling will provide a link between our project and the MHD community. On the gyrokinetic side, we will investigate alternative solution paths, such as the moment-equation based approach, the Maxwell-Vlasov gyrokinetic formulation based on the electromagnetic fields, and the semi-Lagrangian scheme. We will address potential benefits of these alternative approaches on massively-parallel computer systems and for demanding simulation scenarios. An expert in applied mathematics will contribute to these algorithmic innovations. In the following, we will address the high-level objectives of the TSVV #10.

1. Gyrokinetic electromagnetic turbulence and fast particles

This part of the project will specifically address the Deliverable 1: *"Nonlinear gyrokinetic (GK) electromagnetic simulations addressing the mutual influence of heating-induced fast ions and α particles with turbulence."* Our goal will be to combine gyrokinetic turbulence, fast-particle dynamics, zonal flows, and MHD-type plasma response within the same numerical framework. These aspects have been considered so far separately. However in reality, they co-exist and mutually-interact in burning plasmas. We will employ global gyrokinetic simulations to address this physics in all its richness and complexity focusing on the changes in the turbulent dynamics and fluxes (turbulence suppression) induced by the fast particles in the global simulation context. Concretely, the ORB5 and EUTERPE codes will be used in tokamak and stellarator geometries for electromagnetic turbulence simulations in the presence of fast particles. One of the important tasks of the proposed TSVV project will be to refactor these two codes aiming at a European standard code for gyrokinetic particle-in-cell simulations. Further comparisons with other global codes, such as GTC, MEGA, global GENE, GYSELA, GEMPIC-AMReX, and XGC, will be undertaken. The topics of interest will include long-time numerically-stable simulations of turbulent burning plasmas, development of a new gyrokinetic solver formulated in terms of electromagnetic fields (in contrast to the usual formulation using the electromagnetic potentials), and a mathematically-correct formulation and implementation of the gyrokinetic models based on gyrokinetic moment equations and numerical closure for burning plasmas. ORB5&EUTERPE will generate high-fidelity simulation data which will be combined with low-fidelity reduced models for energetic-particle dynamics providing a multi-fidelity input for the integrated transport and MHD stability modelling of burning plasmas. The possibility to prescribe a given time-dependent external perturbation in the ORB5 code will be exploited to disentangle the complex couplings between bulk species, fast ion population, turbulence, zonal flows and global modes.

On the technical side, we will

1) Refactor ORB5 and EUTERPE aiming at a unified framework
2) Port EUTERPE to a new hardware (GPU-based); ORB5 is already GPU-enabled
3) Make ORB5&EUTERPE output IMAS-compatible

SMART (Specific Measurable Assignable Realistic Time-related) deliverables:

Dec. 2023:

(S) Perform global gyrokinetic simulations of electromagnetic (EM) turbulence for a realistic beta in cyclone-based geometry including fast particles in the EM-ITG, KBM, and microtearing regimes. Consider alternative schemes for solving nonlinear EM gyrokinetic equations in the presence of global modes and fast particles. The first scheme will be based on the gyrokinetic moment fluid-like equations with the closure computed numerically as appropriate moments of the gyrokinetic distribution function. The second scheme relies on the formulation of the gyrokinetics in terms of the perturbed fields replacing the more commonly used potentials (synergy with TSVV Task 4, see Section 8).

(M) Demonstrate ORB5&EUTERPE ability to achieve EM turbulence saturation using the standard pullback mitigation scheme.

(A) The work will be done by A. Biancalani, A. Bottino, T. Hayward-Schneider, A. Mishchenko, L. Villard, A. Koenies, R. Kleiber, M. Sadr, E. Poli, M. Campos Pinto, C. Slaby, and J. Graves.

(R) The saturation of EM turbulence is an issue for all gyrokinetic codes; it is challenging and ambitious. At the moment, we have no problems with low-beta EM simulations. They saturate in our simulations due to the zonal-flow excitation. This process has already been intensively studied, also in the presence of fast particles. Extending these simulations to a higher-beta regime may require increased resolution if the zonal-flow generation is not the right mechanism at larger beta (since the Reynolds stress and the Maxwell stress cancel in the Alfvénic state). The physics of EM turbulence saturation is not well studied yet in context of gyrokinetic simulations making this deliverable both interesting and risky. We note that a firm control of the EM turbulence is mandatory for our program as it sets the “scenery” where the global modes develop in presence of the fast particles. We will also consider moment-equation based and Maxwell-solver based techniques, mentioned in this proposal, as alternatives for the high-beta turbulence simulations. These schemes could have an advantage of better scalability due to locality of the solver. This can be important on future exascale computer systems.

(T) We will have clarity regarding this deliverable by the end of 2023 (Dec. 2023). If successful, we will continue EM turbulence simulations in the following years of the project, extending them to ITER and stellarator reactor (e. g. HELIAS) geometries.

Dec. 2025:

(S) Apply all techniques available to this point to burning plasmas in ITER and HELIAS.

(M) Clarify how the EM microturbulence is affected by a large population of fast particles and global modes in burning plasmas.

(A) The work will be done by A. Biancalani, A. Bottino, T. Hayward-Schneider, A. Mishchenko, L. Villard, A. Koenies, R. Kleiber, M. Sadr, E. Poli, M. Campos Pinto, C. Slaby, and J. Graves.

(R) Simulations of reactor-scale plasmas is computationally very expensive. This makes this deliverable risky. However, this is the ultimate goal of our proposed TSVV. It will be doable if we make good progress at the earlier stages of the project with our algorithms, gather an appropriate simulation experience, and adapt our unified ORB5&EUTERPE framework to cutting edge computer systems. Reduced models and hybrid-MHD simulations will be used to define physically interesting cases and compare the simulation results.

(T) We will be able to report on this by the end of 2025 (December 2025).

2. Simulations of global modes and fast-particle interaction

This part of the project will specifically address the Deliverable 2: *"Linear and nonlinear simulations (e.g., GK, extended-MHD, and/or hybrid-MHD-GK) addressing the mutual influence of MHD/EPM and fusion α's as well as suprathermal particles dynamics (also including energetic particles originating from heating sources)."* This topic is naturally included into the unified ORB5&EUTERPE gyrokinetic framework. Indeed, separation of the global nonlinear gyrokinetic solution into turbulence, zonal flows, global modes, fast-particle phase-space structures is possible and meaningful. However, all these components coexist mixed in the perturbed electromagnetic field and distribution function evolution provided by gyrokinetic codes. In the previous section, we have already described the basic steps which we plan for the gyrokinetic ORB5&EUTERPE framework. This activity will be supported and extended by the hybrid MHD-gyrokinetic codes HMGC and HYMAGYC. These codes solve the gyrokinetic equation for fast particles whereas the bulk plasma is treated as a fluid. For this fluid part, HMGC solves reduced nonlinear visco-resistive MHD equations while the MHD module of HYMAGYC (an initial-value version of MARS) solves linear resistive full MHD equations. Moreover, HYMAGYC, being developed within WPCD, is almost fully IMAS-compliant. In particular, it is fully IMAS-compliant for the MHD part; the IMAS compliance of the HYMAGYC gyrokinetic module will be completed within our TSVV project. This experience will then be used to make ORB5&EUTERPE IMAS-compliant. Besides these points, comparing results obtained by the hybrid- and fully-gyrokinetic codes will be of pivotal value for the Verification part of our TSVV project. Currently, the benchmark activities on the NLED AUG testcase are carried out in the frame of the ENR MET project, involving MEGA, ORB5, and HYMAGYC codes. This quite fruitful and interesting benchmark will be continued and expanded to ITER geometry in the proposed TSVV project. On the theoretical side, evolution of the zonal structures in the fast-particle phase space will be analytically described and compared with simulation results. Finally, there are fluid modules in ORB5&EUTERPE, too. This makes a more explicit comparison of ORB5&EUTERPE results and numerical schemes with the results and methods of the hybrid-gyrokinetic codes possible. These fluid modules of ORB5&EUTERPE will be used to implement an alternative fully-gyrokinetic solver based on the gyrokinetic moment equations. We will employ numerical closure relations formulated as appropriate moments of the gyrokinetic distribution function. The knowledge of the distribution function will be needed only for the closure. The perturbed fields will be solved from fluid-like moment equations. There will be freedom to decide if only the fast particles are kinetic, or both the fast and the bulk ions, or all species including electrons. This approach will give us hybrid-gyrokinetic functionality integrated into the unified ORB5&EUTERPE framework and, in addition, an alternative moment-equation based approach for solving the fully-gyrokinetic electromagnetic problem including the drift-wave turbulence. This alternative solver may have advantages with respect to the standard way of solving the quasineutrality equation for the electrostatic potential and Ampere's law for the magnetic potential. All hardware-related developments (GPU etc.) and algorithmic developments (e.g. improving the solver) in ORB5&EUTERPE will be available within this unified framework.

SMART (Specific Measurable Assignable Realistic Time-related) deliverables:

On the gyrokinetic side, all the SMART deliverables described in the previous section apply to this section on equal footing. The deliverables for the hybrid-gyrokinetic part are

Dec. 2023:

(S) Verify and validate the hybrid-gyrokinetic set of the codes.
(M) Finish the NLED-AUG benchmark (code verification) and compare the results to the ASDEX-Upgrade experiments (code validation).
(A) This work will be performed by G. Vlad, Ph. Lauber, A. Koenies, R. Kleiber, L. Villard, M. Sadr, A. Biancalani, and J. Graves.
(R) This deliverable is not very risky but it requires careful and tedious work.
(T) The results of the V&V will be available in December 2023.

Dec. 2025:

(S) Study the role of phase-space structures in ITER plasmas.
(M) Perform HMGC and HYMAGYC simulations of ITER plasmas employing Hamiltonian diagnostics and using theoretical information on the phase-space structure evolution.
(A) This work will be done by G. Vlad, S. Briguglio, F. Zonca, and T. Hayward-Schneider.
(R) This deliverable is not very risky but it requires careful and tedious work.
(T) The results of this work involving theory, simulations, and experiment will be reported in December 2025.

3. Coupling of MHD and gyrokinetic codes with a transport code

This part of the project will specifically address the Deliverable 3: "*Coupling of an extended-MHD/hybrid-MHD-GK code with a transport code to address self-consistently the mutual influence of MHD/EPM driven by fusion α's as well as suprathermal particles and corresponding repercussions on respective deposition profiles and, finally, on bulk density and temperature profiles evolution.*" As mentioned in the previous section, we plan to extend the IMAS compliance to the gyrokinetic module of HYMAGYC and then use this experience to make also ORB5&EUTERPE IMAS-compliant. In addition to this, we will add reduced models of the energetic-particle dynamics, such as the critical-gradient model (CG) [R. Waltz et al, NF **55**, 12 (2015)], and quasi-linear (QL) or kick-like models [M. Podesta et al, NF **56**, 11 (2016)], to a transport code via IMAS.

SMART (Specific Measurable Assignable Realistic Time-related) deliverables:

Dec. 2023:
(S) IMAS compliance of the gyrokinetic hybrid codes.
(M) Make the gyrokinetic module of HYMAGYC IMAS-compliant.
(A) This work will be performed by G. Vlad and J. Ferreira.
(R) This deliverable is not very risky but it requires careful and tedious work.
(T) The fully IMAS-compliant HYMAGYC will be available in December 2023.

Dec. 2025:
(S) IMAS compliance of fully gyrokinetic codes.
(M) Make the ORB5&EUTERPE framework IMAS-compliant.

(A) This work will be performed by A. Bottino, T. Hayward-Schneider, and J. Ferreira.
(R) This deliverable is not very risky but it requires careful and tedious work.
(T) The IMAS-compliant ORB5&EUTERPE will be available in December 2025.

4. MHD stability in presence of a large fusion alpha population

This part of the project will specifically address the Deliverable 4: "*Investigation of the role of a large population of fusion α's, as well as of other suprathermal particles, on the global MHD stability limits of the plasma (e.g., impact on the global β-limit of the kinetic stabilization of the low-n kink modes, or determination of the sawtooth period by inclusion of kinetic effects).*" We will include the effects of shear Alfvén waves on the fast-ion distribution function in extended-MHD simulations. It is known that the fast-ion distribution function can be changed substantially by Alfvén waves. This may modify the way how the fast ions interact with the kink instabilities and affect the sawteeth period. Also, the safety factor and magnetic shear can be changed by the Alfvén waves if zonal currents are generated. On the other hand, evolution of the safety factor during the sawtooth cycle will change Alfvén continuum, Eigenmodes, and their interaction with the fast particles. We will address this complex dynamics in a self-consistent way. As mentioned in the previous section, we will develop reduced CG/QL models describing the evolution of the fast-ion distribution function and pressure profile due to the shear Alfvén waves in our proposed TSVV project. The resulting energetic-particle pressure tensor and transport coefficients will be included into the extended-MHD codes (such as the XTOR code family). We will investigate fast-particle effects on the kink-mode stability and the sawteeth dynamics in the presence of Alfvénic activity. Modifications of the safety factor, Alfvén continuum, and fast-particle profiles caused by sawteeth dynamics will be considered, as well as the resulting effect on the fast-particle interaction with the Alfvénic waves. In this case, the MHD evolution will affect self-consistently the Alfvénic stability, and as a consequence, the result of the reduced modelling. The work on the IMAS compliance, mentioned in the previous section will be of crucial importance for this part. Finally, fully gyrokinetic simulations of kink modes will be addressed using ORB5&EUTERPE, as it has already been discussed above. This problem is closely connected to a more general question of system-scale MHD behavior in gyrokinetic codes. We will consider what is needed in terms of the gyrokinetic formulation and implementation to get the long wavelength motion right.

SMART (Specific Measurable Assignable Realistic Time-related) deliverables:

Dec. 2023:

(S) Linear kink stability in the presence of fast particles and Alfvén Eigenmodes.
(M) Linear and nonlinear hybrid-MHD simulations (XTOR) of internal kink modes in the range of a single sawtooth period in the presence of Alfvén Eigenmodes and fast particles; linear fully-gyrokinetic simulations (ORB5&EUTERPE) of internal kink modes in realistic tokamak and stellarator geometries.
(A) The work will be done by R. Dumont, H. Luetjens, X. Garbet, J. Graves, L. Villard, A. Koenies, R. Kleiber, A. Mishchenko, and A. Biancalani.
(R) The novelty is to combine Alfvén Eigenmode and kink mode simulations within the same hybrid-MHD framework together with the fast-particle evolution. So far, these instabilities have largely been considered separately, e. g. the Alfvén Eigenmode stability by HMGC and the kink stability by XTOR or VENUS-LEVIS. For the fully-gyrokinetic part, linear gyrokinetic simulations of kink modes in tokamak and stellarator geometries have already been performed with ORB5&EUTERPE. For this deliverable, we will apply this capability to ASDEX-Upgrade

and W7-X. The simulations may become numerically challenging in realistic magnetic geometry. This is the risky aspect of this deliverable.
(T) This work will be done by December 2023.

Dec. 2025:

(S) Nonlinear kink stability in the presence of fast particles and Alfvén Eigenmodes.
(M) Nonlinear hybrid-MHD simulations of sawtooth oscillations with the XTOR code family including fast ions and using the pressure tensor provided by the reduced models of the fast-particle evolution in the presence of Alfvénic modes; nonlinear fully-gyrokinetic simulations of internal kink modes using ORB5&EUTERPE.
(A) The work will be done by H. Luetjens, X. Garbet, J. Graves, P. Lauber, A. Koenies, A. Mishchenko, and A. Biancalani.
(R) Nonlinear hybrid-MHD simulations of sawtooth oscillations can be complicated. Nonlinear fully-gyrokinetic simulations of kink instabilities have never been done for realistic burning-plasma parameters and can require large resolution and substantial computation resources. The perspective is the global-gyrokinetic simulations of MHD modes evolving together with the turbulence and fast particles within a single numerical framework in a realistic magnetic geometry.
(T) We will report on this deliverable in December 2025.

5. Burn control and energy deposition optimization strategies

This part of the project will specifically address the Deliverable 5: "*Exploration of active strategies to optimize the deposition of α particle energy, aiming at a maximization of the fusion power yield (e.g., α channeling for a direct ion heating); modelling of burn control through auxiliary heating and fuelling strategies; prediction of current profile, particularly in predominantly ohmically driven scenarios, consistent with bootstrap contributions from pressure profile and fast particles.*" For this deliverable, we will employ integrated modelling for burning plasmas with a focus on the energetic particle physics, in particular using the ETS. In the previous sections, we have described our plans regarding the reduced models, fully-gyrokinetic simulations, hybrid-gyrokinetic and extended-MHD simulations of burning plasmas, integrated in the frame of our TSVV project into a single system through the IMAS interface. This information will be used for further transport simulations taking specific burning plasma aspects, such as the fast-particle interaction with shear Alfvén waves and MHD modes, into account. The main contribution of our project will, however, be the integration of the burning-plasma specifics into an IMAS compatible module which can then be used by other IMAS workflows (ASTRA, OMFIT, METIS, ETS, TRANSP). The emphasis in the first years will be more on the development of our tools, such as the refactoring of EUTERPE&ORB5 as well as the formulation and implementation of the reduced models. The later years of the project will be more focused on integration and applications. We will study burn control including control of thermal instabilities in tokamak and stellarator reactor plasmas. We will consider effect of the alpha-particle dynamics and their interaction with the shear Alfvén waves before they slow-down on the energy deposition profile. This profile will differ from the alpha-particle birth profile which, however, is frequently used in calculations. For stellarator reactors, we will consider how the stellarator-specific transport regimes and scaling of the transport coefficients affect the thermal stability of burning stellarator plasmas and how the available actuators have to be applied. In addition, inherent steady-state operation of a stellarator reactor will be addressed taking different stellarator-optimization concepts into account. Here, we expect synergy and cooperation with the respective EUROfusion Work Packages and TSVVs, and, internationally, with activities such as the Simons Collaboration on Hidden Symmetries and

Fusion Energy. In the early phase of the project we will make first steps to couple the critical-gradient and quasi-linear models (CG/QL), which can quickly be developed in our proposed TSVV project, to the transport code (ETS) via IMAS interface. This will give a chance for other transport codes to experiment with this early implementation using the same data structures and format.

SMART (Specific Measurable Assignable Realistic Time-related) deliverables:

Dec. 2023:

(S) Couple simple reduced energetic-particle (EP) models to the transport solver (ETS) using the IMAS interface.
(M) Perform time dependent transport simulations with reduced EP transport models to explore the influence of AE stability on burn-up physics.
(A) This work will be done J. Ferreira, Ph. Lauber, and J. Graves.
(R) This deliverable relies on the availability of reduced fast-particle models. The simplest CG/QL and kick models are already available in the community.
(T) This deliverable will be reported in December 2023.

Dec. 2025:

(S) ITER burning-plasma ETS simulations using reduced fast-ion models.
(M) Perform extensive burning-plasma scenario studies using ETS and the most efficient fast-ion transport models coupled through an IMAS interface.
(A) This work will be done by F. Zonca, P. Lauber, R. Dumont, and J. Ferreira.
(R) This deliverable relies on success of the previous stage (model coupling to ETS).
(T) This deliverable will be reported in December 2025.

6. Reduced models for AE/EPM stability and nonlinear dynamics

This part of the project will specifically address the Deliverable 6: "*Reduced AE/EPM stability and nonlinear dynamics models for use in predictive and systems codes, aiming, e.g., at predicting tritium burn-up rates and core plasma helium content*". In order to address these questions, we propose to couple simplified energetic-particle (EP) transport models with low fidelity and short evaluation time to transport codes such as ETS. In particular, we will start with the implementation of a critical gradient (CG) model based on local analytical and numerical estimates for stability boundaries and mode structures. We plan to use the IMAS-compatible linear gyro-kinetic LIGKA code for this purpose. This model will deliver marginal EP profiles that can be used e.g. for burn-up studies. (Note, however, that the crucially important intermittency of EP transport cannot be addressed with a CG model.) Since the model depends on a simple "recipe" for the onset of considerable EP transport above the linear stability threshold [R. Waltz et al, NF **55**, 12 (2015)], the CG model should be tuned with a quasi-linear or a kick model similar to [M. Podesta et al, NF **56**, 11 (2016)]. The HAGIS/LIGKA framework can deliver the necessary building blocks for the construction of a phase-space resolved diffusion coefficient similar to the methodology of the original kick model. However, this model already requires considerable computing resources. It has to be explored if a kick model will be considerably faster than an optimized nonlinear single-mode HAGIS/LIGKA run. An advantage of the HAGIS-LIGKA framework is that it supplies a consistent estimate for the mode saturation amplitude. In the kick model, the saturation amplitude is a free parameter to be provided by the experiment or a quasi-linear/non-linear model. The models above will be implemented within the IMAS framework. This ensures that more advanced models (not part of this proposed TSVV) can easily be adopted in the future since all reduced EP models rely on the critical infrastructure which we plan to address in a first step. This work will include the implementation, the verification and the validation of an automated EP stability workflow on the selected scenarios (see Section 7). The necessary codes and libraries will be made available on the EUROfusion Gateway. Since the automatic determination of damping and drive is very crucial and still challenging (also computationally) due to global and non-perturbative effects, this task will require considerable resources, especially when applied to different experiments and scenarios. Following steps can be identified:

1. It is clear that the quality of the final transport model will critically depend on the EP physics workflow. Therefore, it has to be well tested, exception handling and failure treatment has to be implemented (milestone end 2022). Despite their physical insufficiency, simple models, such as the CG model, are well suited as a testbed for this work and for gaining experience with the challenges of time-dependent couplings.
2. Development of a more advanced kick-model-like approach will be the milestone for 2023 although the kick-model per se is not predictive with the amplitudes being free parameters. The HAGIS/LIGKA model delivers these non-linear amplitudes more consistently albeit neglecting wave-wave non-linearities, collisions and turbulence.
3. This deficit can further be mitigated using results from more consistent codes: collisions with CKA-EUTERPE, wave-wave nonlinearity with HYMAGIC, wave-wave nonlinearity and turbulence with ORB5 and EUTERPE. This will lead to a more advanced model compared to the original kick-model [M. Podesta et al, NF **56**, 11 (2016)]. Development and validation of this models will be a milestone for 2024; further application and optimization will be done in 2025.

It is important that the infrastructure and experience gained during this sub-tasks can be transferred to the implementation of future, more advanced models, which can be predictive on much longer time scales of the order of the energy confinement time. These models require a different and more fundamental first-principle-based approach, and a corresponding different project team. We believe that this openness to alternative and future developments will be a strength of our proposal.

<u>SMART (Specific Measurable Assignable Realistic Time-related) deliverables:</u>

Dec. 2023:

(S) Implementation of a critical gradient model into the transport solver (ETS). Explore the performance of kick-like models compared to nonlinear single mode runs (HAGIS/LIGKA).
(M) Perform basic ETS studies using CG/QL models included through an IMAS interface.
(A) This work will be done by Ph. Lauber, J. Ferreira, and J. Graves.
(R) Technical details (e. g. the underlying equilibrium representation and distribution function interface) have to be resolved. Based on previous experience, no major risks are expected.
(T) This deliverable will be reported in December 2023.

Dec. 2025:

(S) Implementation of phase-space resolved fluxes into the transport solver (ETS), as given by the kick model or more advanced nonlinear computations or models.
(M) Compare the performance (accuracy vs. speed) of time dependent transport simulations with phase-space resolved EP transport models to the CG model.
(A) This work will be done by Ph. Lauber, F. Zonca, R. Dumont, and J. Ferreira.
(R) Optimal strategies for time dependence of the couplings between the EP transport model and the transport code have to be developed.
(T) This deliverable will be reported in December 2025.

7. Validation plan

During the whole project time, we plan to validate continuously the available codes and models with experimental data. We propose to choose a set of reference scenarios from different present-day and near future experiments. These scenarios will be relevant for various sub-aspects of the validation, such as magnetic geometry, finite-beta effects, heating methods, or types of the EP transport regimes, based on the following pre-existing elements:

1. Experience from past EUROfusion ENR projects (NLED, NAT, MET): reference cases are available for ASDEX-Upgrade, DDT, JT-60SA, and ITER; see the project websites [https://www.afs.enea.it/zonca/METproject/] and [http://www2.ipp.mpg.de/~pwl/]. Many of the codes contributing to TSVV#10 have already been validated for both the linear onset and the non-linear evolution of EP driven instabilities and the related transport. References to the publications and presentations describing these cases are available on the project websites.
2. The recent application of LIGKA/HAGIS (A. Bierwage & Ph. Lauber, see recent ITPA-EP meeting, various JET TF meetings) to JET (DTE2: Extrapolation from D-3He) will be used as a starting point for the further investigation of alpha particle physics at JET. The future strategy will be discussed and adopted in agreement with the JET TF leaders.
3. Predictive modelling of JT-60SA and validation on old JT-60U data has been a topic bridging WPSA and ENR (NAT, MET) efforts. This project will be continued within TSVV/WPTE (Ph. Lauber, J. Ferreira) including AE stability analyses based on DDT projections, which will be further evolved and detailed.

Starting from these already existing efforts, we propose, in close connection with WPTE task force leaders, the following next steps and tentative workplan:

1. Review the scenarios and update them in case this is found to be necessary (milestone 2021); presently ongoing efforts will be finished; various publications in 2021, in particular in connection with IAEA FEC 2021 can be seen as a first milestone.
2. Formulate reference cases for fast-particle effects in W7-X for ICRH three-ion species scenario in a low-density plasma discharge and for a combined ICRH/NBI heating scheme (in cooperation with WPW7X). This will not only allow studying AE stability in W7-X for the different heating schemes but also comparison of the fast-particle effects in tokamak and stellarator geometries. The stellarator tools validated on these reference cases can later be used to study 3D effects in tokamaks.
3. Add time-dependent reference cases to test EP stability and transport workflows. This requires more time since many experiments are not ready to provide IMAS compatible output, nor the necessary tools e.g. to automatically smooth profiles and adopt them for simulations. In particular, also the further development of heating and current drive codes (not part of this TSVV) needs to be taken into account. It is expected that first time-dependent IMAS data with simplified fast-particle distribution functions will be available in 2022, whereas more sophisticated cases will be added in 2023 and later.
4. Propose new EP-related experiments that the TSSV#10 personnel finds to be most critical and useful for the code validation. Again, this will be carried out in close connection with the respective TF leaders at various experiments. Since this requires more preparation, we expect first dedicated experimental data in 2022/23.
5. Choose a DEMO relevant scenario, based on the needs and results of the EUROfusion DEMO team. Since there are still uncertainties about the most relevant regimes, this work is foreseen towards the end of the TSVV#10 lifetime.

Finally, sensitivity to profiles (safety factor, density, temperature, etc.) is a major difficulty in the EP modelling. In fact, it is one of the most critical aspects to be addressed when moving from validation to prediction. For this crucial aspect, the advantage of having a set of hierarchical codes that are the back-bone of our proposal becomes very obvious. After understanding the physics of a certain reference case as delivered by the model hierarchy, the cheaper codes can be used for a wider exploration of the parameter space without losing confidence in the results. This saves computational resources that can be dedicated to the most challenging simulations. It should be noted, that there are no sufficient resources in the TSVV program to provide detailed and specific modelling for all relevant EUROfusion experiments and discharges. Instead, we propose to deliver the tools (once tested and results published), input files for specific cases, and a support to a limited set of EP experts outside the TSVV group. As an organisational aspect, we propose to have regular meetings (twice a year, or, on request, on shorter notice) with the Leaders of WPTE, WPJET, and WPW7X.

8. Synergy with other TSVV Tasks

Development of gyrokinetic codes is one of the important goals of our proposal. In this respect, we expect a very natural collaboration with two other TSVV Tasks which have a strong gyrokinetic component. First, we have an overlap with Task 1 which also includes ORB5 simulations in its program. Naturally, further development and applications of this code planned within Task 10 will be of immediate interest also for the TSVV Task 1. In fact, ORB5 applications in Task 1 are related to the core-edge coupling (implementation of boundary conditions, profile evolution, radial electric field evolution) whereas the proposed Task 10 focuses on the core EM applications (EM turbulence in presence of global modes and fast particles). After a separate development of these different capabilities in the two Tasks, we expect to combine this work approaching this way the goal of the full-device modelling and extending the burning plasma simulations to the pedestal region (2025+ phase). Another possible overlap is with the TSVV Task 4 which develops GEMPIC-AMReX code for edge applications. The novel formulation of GEMPIC-AMReX is based on the electromagnetic fields replacing more conventional potentials. This approach may be of interest also for burning-plasma applications requiring long-time numerically-stable simulations of electromagnetic turbulence. The advantages of this formulation compared to the standard one are the absence of the cancellation problem and, eventually, a better scalability due to locality of the solver. This could make GEMPIC-AMReX especially attractive on future exascale systems. We are interested in this work done by Task 4 and propose to support it providing physics application cases in the electromagnetic regime. PICLS is another code developed within Task 4. This particle-in-cell code for edge application is a close relative of ORB5/EUTERPE. These projects will eventually merge in the future. In terms of ACH resources, GPU extension planned for ORB5 solver and EUTERPE will generate experience and tools which will help GPU-enabling of other codes, such as GYSELA, GENE, GEMPIC-AMReX, etc., implemented eventually by the same ACH. Similarly, performance optimization of GEMPIC-AMReX (ACH resource requested by Task 4) will facilitate this kind of work for ORB5&EUTERPE. Also, visualization and IMAS support (for example, for ORB5), proposed in Task 1, will generally be applicable and used in the proposed here Task 10. On the organizational side, the PIs of the proposed TSVV Tasks 1, 4 and 10 agreed to meet on a regular basis (quarterly) to discuss all these mutual developments and coordinate efforts.
Synergies with other TSVV Tasks are also possible. For example, Task 12 will provide optimized stellarator configurations which can be tested with respect to the plasma ignition and fusion burn. Such tests could be done using the tools developed in our proposed TSVV Task 10. Also, Task 13 could benefit from EUTERPE developments in our proposed Task since EUTERPE is used in Task 13 to simulate the stellarator turbulence. Finally, Task 11 is

dedicated to integration of all reduced models developed in the TSVV program including our proposed Task 10. Investments into the development of IMAS and ETS eventually planned in Task 11 will be important for all other Tasks integrating reduced models, including Task 10.

9. Summary

In summary, we list main project's milestones including the management plan and risk assessment. Further details on the program milestones and the team members involved into the various work packages can be found in the description of the SMART deliverables provided for each project's high-level deliverable in the text above.

Milestone/work package	Management plan	Risk assessment
Implementation of reduced fast-particle and Alfvénic physics models	1. Review critical-gradient and quasi-linear models (2021). 2. Define the simulation loop and the codes required to implement the models (2022). 3. Implement the models using IMAS interface between the codes (2023).	Combining several codes together can be tedious because of the differences in the output format, coordinate systems, etc.; IMAS format is supposed to mitigate this risk.
Coupling of reduced fast-particle models into the integrated-transport framework (ETS)	1. Review the integrated modelling loop describing burning plasmas including effect of Alfvénic modes (2021). 2. Establish IMAS interface between different parts of the integrated modelling loop (2022). 3. Integrate reduced fast-particle and Alfvénic physics models into the modelling loop (2023).	The problem of code coupling is a risk, to be mitigated by IMAS. There could be missing parts, e.g. related to the distribution function generation.
Fully-gyrokinetic global simulations of electromagnetic turbulence and zonal structures in the presence of global modes and fast particles for realistic burning-plasma parameters (ORB5&EUTERPE)	1. Perform simulations of EM turbulence in presence of fast particles using existing codes increasing plasma beta and size (2021). 2. Perform gyrokinetic simulations of MHD modes (kink and tearing) increasing plasma size and temperatures (approaching burning plasma conditions) (2022). 3. Combine turbulence, fast particles, zonal flows, and global modes under burning plasma conditions (2023).	Gyrokinetic model combines disparate scales; it is to be clarified if this combination can be handled numerically at a reasonable computation cost. Availability of the HPC resources and ability of the codes to use this resources is another risk. Risk of code adaptation to new hardware will be mitigated by ACHs.
Validation of burning-plasma simulation tools using experimental data (JET,ASDEX-U,JT-60SA, W7-X)	1. Review the existing EP validation scenarios and update them in case this is found to be necessary (2021). 2. Define time-dependent reference cases for different machines (2022). 3. Initiate new EP-dedicated experiments and choose scenarios relevant for ITER and DEMO (2023).	Time-dependent reference case will rely on successful IMASification on both EP and non-EP parts (equilibrium, current drive, heating, fueling, etc.). The validation experimental data should be sufficiently complete and of good quality. EP-dedicated experiments are desirable.

Expected High Performance Computing requirements

The most expensive part of the project will be related to the gyrokinetic simulations of electromagnetic turbulence and global modes in the presence of fast particles in tokamak and stellarator geometry. To estimate the amount of the computer resources needed in the early phase of the project, we can use the OrbZONE, ORBFAST, EUGY, and HYMHDGK3 projects dedicated to simulations of this type and ongoing on the Marconi-Fusion supercomputer. The total amount of node hours requested in these projects is 3 587 000 for the nodes equipped with the conventional processors (Marconi SKL) and 160 000 for the non-conventional GPU-based nodes (Marconi100). Given a larger scale of the proposed TSVV project, we would like to increase the amount of the node hours to 4 000 000 per year on the conventional nodes and to 700 000 node hours per year on the GPU-based nodes. Note that ORB5 is GPU-enabled and shows a very good scaling on Piz Daint and Summit. It is currently in active use on Marconi100. EUTERPE will be GPU-enabled soon using the ACH component of our proposed TSVV project, as described in the next section. In terms of the node number requirement, we need from 24 (ORB5) to 64 (EUTERPE) conventional nodes and from 32 to 64 GPU-based nodes (Marconi100) for the electromagnetic turbulence simulations.

Support – in terms of nature and level – to be provided by the Advanced Computing Hubs

One of the key goals for our proposed TSVV project is to address the cross-scale aspect of burning plasmas: micro-turbulence co-existing with the large-scale MHD-like disturbances, radial profile evolution (related for example to the zonal flows), and in the presence of the energetic particles. Global PIC codes provide an excellent framework for the full-device long-time cross-scale modelling of fusion plasmas in general magnetic geometry (both tokamaks and stellarators). Such codes belong to the domain of High Performance Computing and require large supercomputer systems to run on. This technology becomes increasingly complex caused by the transition from the traditional homogeneous to new heterogeneous architectures which rely on various special hardware (GPUs etc.) in addition to the conventional CPUs. This creates challenges for supercomputer centers, compiler and numerical library vendors, as well as developers of application codes. The crucial role played by the new hardware in the future of computing will have a profound effect also on the basic algorithms used by the gyrokinetic PIC codes, which will have to be adapted to massively-parallel code execution. This new situation calls for a centralized framework for further development of gyrokinetic PIC codes targeting the full-device long-time cross-scale modelling of tokamaks and stellarators. In our project, we will address this by refactoring of the global gyrokinetic PIC codes ORB5 (tokamak) and EUTERPE (stellarator) aiming at providing a common platform for both codes. This will serve as a platform for further development and integration targeting the full-device long-time cross-scale modelling in general magnetic geometry.

Development of this unified GK PIC framework starting from ORB5 and EUTERPE will be the focus of ACH work associated with this proposed TSVV project. We will have to enhance the modular structure of these codes introducing new data structures tailored for the heterogeneous hardware, such as the "Larmor" data structure of ORB5, and, generally, establish a more modern approach to the data exchange in the codes (getting away from the "globals"). We will need experts on the new architecture (GPGPUs) to implement the data structures and

code layout required for the emerging hardware and for a practical implementation of the kernels on a given hardware using a directive-based (OpenACC, OpenMP4.5/5.X) or library-based (Kokkos) approach. Introducing new data structures and making EUTERPE and ORB5 more modular and flexible will simplify the exchange of modules between ORB5 and EUTERPE leading to the unified framework in a natural way. The modular data-centric structure of the resulting framework will simplify the implementation of new numerical algorithms. One non-exclusive example is the gyrokinetic Maxwell solver, mentioned in the previous sections, giving us an alternative formulation of the electromagnetic gyrokinetics based on the electromagnetic fields free of the cancellation problem, in contrast to the usual formulation of the gyrokinetic theory based on the electromagnetic potentials. The resulting field solver will be local in space which is optimal for massively-parallel computer systems provided by EUROfusion. Finally, ACHs will support the code technical infrastructure: Git server, Jenkins, simulation data server, as well as special libraries for parallel HDF5 output, linear algebra, and finite elements. Integrated modelling and IMAS compliance may require dedicated ACH support, too. For the five-year period of 2021-2025, our proposed project will request 84 PM of ACH support (High Performance Computing) for the GPU-enabling and code performance optimization; 84 PM of ACH support (High Performance Computing) for the development of scalable PIC algorithms; 12 PM of ACH support (Integrated Modelling and Control) for the IMAS adaptation and reduced-model integration.
Practically, we will start with introducing the Larmor data structure into EUTERPE and getting rid of globals in EUTERPE and ORB5. Once this is done, the implementation of OpenACC/OpenMP directives in EUTERPE will be basically a copy/paste from what already exists in ORB5 giving us a fast route to a GPU-enabled EUTERPE. In parallel, a more "aggressive" code modularization and a library-based approach for the GPU part of the code will be introduced. The resulting framework will be further developed aiming at a European standard code for gyrokinetic particle-in-cell simulations.