Proposal for participation in a “Theory, Simulation, Validation and Verification” (TSVV) Task

Title (c.f. Annex-2)	*TSVV Task 6: Impurity Sources, Transport, and Screening*
TSVV Task leader (name/e-mail)	*Dr Guido CIRAOLO, guido.ciraolo@cea.fr*
Lead beneficiary	*CEA (France)*
Project duration	*5 years*

ABSTRACT

The present proposal is the answer from a consortium of European Research Units to the call for participation in the TSVV task number 6 concerning the development, verification and validation of advanced numerical tools in order to predict impurity sources, transport and screening in the edge plasmas of ITER and DEMO fusion devices.

Today state of the art numerical studies of W transport in SOL and edge plasmas of present machines as well as for ITER scenarios mostly rely on 2D axisymmetric approximation, preventing any kind of prediction for the impact of 3D perturbations like RMP on W transport and core contamination. Moreover, seeding impurities are usually considered as traces and modelled using the fluid approach, both assumptions becoming quite restrictive in the case of strongly dissipative scenarios with high Z species like Ar envisaged for next step devices.

To go further and address the key deliverables as stated in the call, the present consortium brings together research teams at the forefront on 3D modelling of edge plasma and impurity transport in realistic wall geometries and complex magnetic configurations, with the use of the state of the art codes SOLEDGE3X, EMC3-EIRENE and ERO2.0. These tools, intrinsically built for performing 3D simulations, are complementary in their approaches allowing to address, for example, both steady state and time dependent scenarios like the loss of semi-detached divertor in ITER, complex magnetic configurations in presence of 3D perturbations, as well as impact of turbulence on radial transport. Moreover, regarding the implementation of 3D kinetic transport model for heavy impurities (including W), the consortium is very well positioned for achieving this goal, having in his hands the above mentioned appropriate numerical tools as well as the experience on multi fluid plasma behaviour. This will be very useful for the interpretation and verification of the results obtained with the new kinetic modules.

Finally, in the call is also required to address kinetic transport of heavy impurities in pedestal region. To such aim, we will rely on state of the art kinetic and gyrokinetic codes as VENUS-LEVIS and GyselaX both of them allowing to model impurity transport in high performance edge plasmas in presence of complex 3D magnetic configurations with magnetic symmetry breaking, taking into account both neoclassical effects and turbulent ones. The longer-term goal is to derive a map for diffusion coefficients and peaking factors for heavy impurities to be implemented in fluid code like SOLEDGE3X in order to have a full-integrated description of W transport, for example, from its sources on the wall up to the top of the pedestal.

Building such complex numerical tools requires constant verification and validation. In the workplan presented in the full proposal these verification steps are detailed as well as the validation one, focused on a few specific experiments, being intended that several other experiments will be also possible in the framework of WP TE /PWIE

The possibility to test in parallel different solutions in existing tools also strongly mitigates the risk associated with making key structural decisions before having a complete feedback on their practical implications in terms of performances, numerical precision or stability.

Note finally that the position of the project at the crossing of several key physics issues for the edge plasma also calls for strong collaboration with other TSVVs, especially TSVV 3 (Plasma Particle/Heat Exhaust: Fluid/Gyrofluid Edge Codes), TSVV 5 (neutral gas dynamics in the edge), TSVV 1 (Physics of the L-H Transition and Pedestals) and 4 (Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes). Close contacts between these projects have already been made in the course of their preparation in order to ensure their consistency and complementarity. Specific effort will be devoted to promoting communication channels between these projects. Since a close team collaboration is foreseen and necessary it should also be noted that mobility support will be needed to allow for at least annual face-to-face and occasional bilateral meetings.

A detailed workplan, a risk assessment, an estimate for the required HPC resources as well as our need for ACH support are stated in the full proposal

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Relevant skills and experiences of the TSVV Task team

Briefly describe the skills and experiences of the TSVV Task team members which are relevant to accomplishing the goals. These skills may also include methodological expertise, say in software engineering, code integration, computer science, HPC code development, or numerical techniques.

Guido Ciraolo: Guido Ciraolo is a senior research scientist at IRFM. He has background in theoretical physics and computational fluid dynamics and he is working on edge plasma physics since more than 15 years. His expertise covers theory and numerical modelling of edge plasma transport and turbulence as well as experimental data analysis and comparison with simulations, in particular on the WEST tokamak. He is one of the main expert of SOLEDGE code and he has been involved in several Enabling Research projects focused on edge and scrape-off layer physics, as well as plasma wall interactions, during the H2020 FP. He has also long experience in scientific team management, having been previously head of the Edge Plasma Physics group and currently head of the Divertor and Plasma wall Interaction group at IRFM.

Hugo Bufferand: H. Bufferand is scientist at CEA, and has a background of aerospace engineer. He is working since his Phd at Aix-Marseille University on fluid plasma solvers, being the main developer of the multifluid transport code Soledge2D and co-developer of the Soledge3X boundary code. He worked closely with Dr. Marandet on the coupling of these fluid solvers to the EIRENE code and on the hybrid model for neutrals. He also has worked on improving the description of the sheath boundary in coupled fluid/kinetic simulations.

Etienne Gravier: Professor at the University of Lorraine, is in charge of the second year of the Master of Science in fusion and plasmas in Nancy, member of the coordinators of the French Research Federation in Magnetic Confinement Fusion, and was head of team “High temperature plasma physics” of the Jean Lamour Institute from 2012 to 2018. He participated on the development of a gyrokinetic code focusing on the trapped particles, which simultaneously describes trapped-ion (TIM) and trapped-electron (TEM) driven modes (Trapped Element REduction in Semi lagrangian Approach, TERESA-4D, sister code of GYSELA-5D). Competition between streamer-like structures and zonal flows has been observed for TEM and TIM turbulence while zonal flows have been shown to play an important role in suppressing nonlinear TEM transport depending on the temperature ratio T_e/T_i. Diffusive transport as well as impurity pinch have been investigated. Recently new results have been obtained with GYSELA regarding the scalings for the impurity diffusion coefficients and the peaking factor with the impurity charge number. Both neoclassical and turbulent transports have been compared. E. Gravier supervised the work of Kyungtak LIM (Univ of Lorraine), who started his PhD in October, 2018 (supervised both by IJL and IRFM). He will supervise the new PhD program dedicated to this project (G. Lo-Cascio, from October, 2020).

Yannick Marandet: Yannick Marandet is a senior CNRS research scientist working at Aix-Marseille University in close collaboration with CEA. He has 15 years of experience with the EIRENE code, first for Tore Supra experiments modelling in the framework of various EFDA tasks, then on the coupling of EIRENE to fluid codes developed at CEA, now fused into SOLEDGE3X. He is working on comparison between code and experiments, in particular on WEST but also on other machines. He was involved in several Enabling Research projects focused on edge and scrape-off layer physics, as well as plasma wall interactions, during the H2020 FP.

Madhusudan Raghunathan: Madhusudan Raghunathan is currently a post-doctoral researcher at Aix-Marseille University, working under the supervision of Dr. Yannick Marandet on collisional kinetic theory and closures for use in fluid codes such as Soledge3X. He obtained his PhD in 2018 under the guidance of Dr. Jonathan Graves at EPFL working on a thesis that investigated heavy impurity ion transport in the presence of a saturated internal kink, which involved neoclassical modelling of 3D friction force and PIC drift-kinetic simulations using VMEC and VENUS-LEVIS with neoclassical additions. He also has experience in fundamental collisional and non-collisional kinetic theory from his Masters' project and from his previous and current post-docs

Derek Harting: Derek Harting is scientist at FZJ and has more than 10 years experience in 2D/3D SOL modelling, HPC development and the application to machines like JET, ITER and W7-X. He is an expert in code-code coupling e.g. for core-edge coupling and coupling of fluid SOL codes to the kinetic Monte Carlo code EIRENE and has a broad experience in code management. He is currently the main developer for EMC3-EIRENE at FZJ and has taken over the responsibility for the kinetic ion transport module of EIRENE.

Juri Romazanov: Juri Romazanov (FZJ) holds the EUROfusion researcher grant on “Massively parallel Monte-Carlo modelling of global material migration taking into account three-dimensional plasma configurations and wall geometries” (until 04.2022) and is the lead developer of the ERO2.0 code with broad experience of code application to JET, ITER, W7-X and DEMO.

Postdoc FZJ: Postdoc to be hired with a background in SOL modelling preferable 3D SOL modelling with EMC3-EIRENE. He / she should also have some experience with scientific code development especially FORTRAN would be beneficial. The Postdoc should support D. Harting with the EMC3-EIRENE related modelling and validation of EIRENE-KIT.

Henri Kumpulainen: Henri Kumpulainen is a second-year PhD students at Aalto University with expertise in interpretation of JET H-mode plasmas for W transport in both the edge and core. He is a user of the JET JINTRAC code, including the ELM models in JINTRAC, EDGE2D-EIRENE, and the trace-ion codes ERO2.0 and DIVIMP. He is familiar with the core and edge diagnostic system of JET to validate JINTRAC and ERO2.0 solutions.

Jon Graves: Jonathan Graves is a senior scientist at EPFL, Switzerland, and Honorary Visiting Professor at the University of York, UK. A member of the EUROfusion STAC, he is recognised as an expert in wide range of magnetically confined fusion physics topics, notably MHD instabilities in tokamaks, RFP's and stellarators, fast particles, kinetic-MHD, ICRH heating and impurity transport. He has directed 9 Ph.D. students, and continues to follow 5 more Ph.D. projects. One completed project investigated heavy impurity ion transport in the presence of a saturated internal kink modes in a rotating tokamak plasma. That work is being improved in a new Ph.D. thesis, taking into account neoclassical toroidal viscosity, and other relevant physics processes. The thesis is also being applied to the fundamental features of impurity transport in ELM free H-modes

Michael Eder: Michael Eder is currently a second year PhD student with an assistant teaching position at the Institute of Theoretical and Computational Physics at Graz University of Technology.
He has already written his Master’s thesis in the field of guiding-center motion, and is the main developer of the guiding-center orbit tracing code *Gorilla*, which is a mesh-based geometric integration method being an order of magnitude faster than conventional integrators while preserving the invariants of motion. Michael has a strong numerical background and in addition experience with

modelling of neoclassical transport in both Tokamak and Stellarator geometries. He has already attended many conferences and summer schools (CCFE, St. Petersburg, Simons/PPPL Stellarator Optimization, EPS 2019). He is focusing in his PhD thesis on a kinetic approach to computation of plasma equilibria in 3D magnetic fields with general topology.

Commitment of the TSVV Task team members during the period 2021-2023, and indication beyond 2023

The table below summarizes the commitment of team members in terms of ppy for each year between 2021 and 2025, with values beyond 2023 being indicative:

Team member	Beneficiary	2021	2022	2023	2024	2025
G. Ciraolo	CEA	0,7	0,7	0,7	0,7	0,7
H. Bufferand	CEA	0,5	0,5	0,5	0,5	0,5
E. Gravier	CEA	0,4	0,4	0,4	0,4	0,4
Y. Marandet	CEA	0.2	0.2	0.2	0.2	0.2
M. Raghunathan	CEA (AMU)	0.5	0.5	0.5	0	0
D. Harting	FZJ	1	0,7	0,5	0,5	0,5
Postdoc	FZJ	0,5	0,5	0,5	0,5	0,5
J. Romazanov	FZJ	0	0,3	0,5	0,5	0,5
H. Kumpulainen	VTT (Aalto Univ.)	0,5	0,5	0,5	0,5	0,5
Postdoc/PhD	EPFL	0	0	0	0,5	0,5
J. Graves	EPFL	0	0	0	0,1	0,1
M. Eder	OEAW (Graz TU)	0,5	0,5	0,5	0	0
F. Reimold	MPG	0	0	0	0	0
ACH resources		1	1	1	1	1
Total		5.8	5.8	5.8	5.4	5.4

Additional notes:
The few exceptions to the rule of 0.5 ppy minimum commitment are justified as follows:

- Professor Etienne Gravier has to stay under 0.5 ppy for French law concerning people with teaching duties. A PhD student, funded by other means, will support him all along the duration of the project.
- Dr Y Marandet is mainly involved as supervisor of the CEA (AMU) postdoc. Moreover the project will benefit from his competencies on physics and modelling of neutrals with the EIRENE code, activity where he is also involved in TSVV 5
- Professor Graves is involved in the project as consultant in the first phase of the project and then at 1pm as supervisor of the EPFL postdoc. Given his outstanding experience and the associated benefit for the project, we believe this to be justified.
- Dr Felix Reimold from IPP Greifswald is also listed as a member at 0 ppy. He has shown strong interest for the project and he will participate as consultant, in particular for the comparison between simulation and experiment results on W7X.

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

The call for TSVV Task 6 lists the three following key deliverables:

1. Validated suite of 3D codes and transport models to describe in an integrated way the W content and its distribution in metallic devices, in particular DEMO and ITER, with discrimination of main chamber and divertor sources, screening, transport, and exhaust along with its impact on the main plasma dynamics and performance.
2. Assessment of the W influx, W screening, and W transport in ITER plasmas envisaged for pre-fusion and fusion power operation with semi-detached divertor and application of resonant magnetic perturbations for ELM suppression. Discussion of the impact on a potential loss of semi-detachment and ELM suppression on the W influx, W screening, and W transport in those ITER scenarios.
3. Applications of the developed model. Assessment of the seeding impurity screening and transport in DEMO and ITER scenarios.

In the following, we propose a detailed workplan presenting for each of these key deliverables a list of milestones and sub deliverables intended to show the temporal progression of the work and to ensure reaching key deliverables by the end of 2025. Before entering in the list of milestones we present the main numerical tools we will use and develop for these purposes.

○ Description of the numerical tools

- **SOLEDGE3X:** SOLEDGE3X is a recently developed multi-fluid boundary code developed at CEA/AMU. It solves 3-moment drift-fluid equations for an arbitrary number of species using a Zhdanov collisional closure. It can be used either as a mean-field code (2D or 3D) or as turbulent code (3D) and is the successor of the SOLEDGE2D [Bufferand 15] and TOKAM3X [Tamain 16] codes. It can handle arbitrary magnetic and wall geometries through the use of mask functions inspired from penalization methods. Neutrals are currently being implemented via a simplistic embedded fluid model as well as kinetically through coupling to the EIRENE code. SOLEDGE3X is parallelized using a multi-level domain-decomposition and typically runs on ~1000 cores.

- **EMC3-EIRENE:** EMC3 [Feng1999, Feng2014] is a 3D steady-state fluid Monte Carlo code which solves a set of fluid equation (particle-, momentum- and energy-balance of electrons and ions) for the main plasma species which can handle complex 3D magnetic topologies including stochastic fields due to resonant magnetic perturbations and 3D wall structures. It is closely coupled to the kinetic neutral Monte Carlo code EIRENE [Eirene] for the source terms of the fluid equations. Both codes (EMC3 and EIRENE) are fully MPI parallelized and typically use for production-runs on the order of 64 cores. EMC3 includes also simplified trace fluid model for impurities with only radiative feedback on the main plasma.

- **EIRENE-KIT:** EIRENE-KIT [Schluck2020] is a kinetic ion transport module embedded in the kinetic neutral Monte Carlo code EIRENE. It is currently under development with emphasis on the coupling to EMC3. The kinetic ions are followed by a guiding centered approximation with anomalous diffusion and gradient-B drifts (including mirror force effects). For coulomb collisions, it currently uses a simplified model by an energy relaxation time approach.

- **ERO 2.0:** is a Monte-Carlo code for predicting the steady-state plasma-wall interaction (PWI) and impurity transport. Due to the trace impurity approximation underlying its transport model, ERO2.0 requires importing of plasma backgrounds as input from edge transport codes like EMC3-EIRENE or SOLEDGE3X. ERO2.0 is a massively parallel upgrade of the original ERO code [Kirschner00, Kirschner16] that allows 3D simulation in the entire plasma edge of a reactor-scale device, using a realistic description of all relevant PFCs (e.g. based on CAD models), with a high level of local geometry resolution. Furthermore, it offers a dynamic model for microscopic morphology effects, such as surface roughness. ERO2.0 was designed for high-performance computing (HPC) and shows excellent parallel scaling on more than 1000 CPU cores [Romazanov17]. The particular advantage of ERO2.0 is the possibility to describe the kinetic transport with full resolution of ion gyro-orbits. In combination with comprehensive models for the sheath potential, the impact energies and angles of particles hitting the wall are calculated, which is essential for estimating the sputtering yields. Furthermore, effects such as prompt re-deposition of heavy ions like W can be accounted for [Kirschner16]. Finally, ERO2.0 offers a range of synthetic diagnostics, such as e.g. wide-angle spectroscopic images, for verification with experimental data, along with utilities for comparison to post-mortem surface analyses, and has been already successfully validated at JET [Romazanov19a] and applied to WEST [Gallo20] and ITER [Romazanov19b].

- **GYSELAX** is the refactoring of Gysela [Grandgirard16] initiated in the frame of several European projects. Its main current modelling capabilities important to edge-SOL modelling include: (i) full-f code regarding gyrokinetic equation, still linearized polarization density in quasi-neutrality equation, (ii) flux-driven code with prescribed versatile sources (matter, momentum, energy, vorticity), (iii) Ion Temperature Gradient (ITG) and Trapped Electron Mode (TEM) turbulence, (iv) linearized multi-species collision operator, valid for arbitrary mass and charge and (v) plasma-wall interaction in limiter configuration using a penalization technique (imported from fluid codes), with adiabatic electrons only so far. Recent publications relevant in the context of this TSVV project are [Gravier17], [Idouakass18], [Gravier19], [Lim20].

- **VENUS-LEVIS:** The VENUS-LEVIS code [Pfefferle14] will be applied to investigate the transport of heavy impurities in the presence of saturated 3D MHD structures at the edge of high performance tokamak plasmas. Of particular interest will be the impact magnetic symmetry breaking associated with in-vessel and ex-vessel coils (using free boundary VMEC - see Ref. [Pfefferle15], and internally generated structures such as edge harmonic oscillations (EHOs, see [Kleiner19]. The work, which extends that of Ref. [Raghunathan17], will self consistently take into account neoclassical toroidal viscosity, centrifugal effects and essential collisional dynamics. Further publications, and a completed Ph.D. thesis, are scheduled for 2021. A limitation of the current approach is that heavy ion self-collisions cannot yet be included. Nevertheless, the unique features of the VENUS-LEVIS code permits an otherwise realistic investigation into the difficulties of sustaining QH-modes in plasmas with a tungsten divertor (due to impurity accumulation in the 3D edge), and the potential impact of EXB flow shear, thermal profiles in the separatrix, and in-vessel and ex-vessel coils.

- **GORILLA:** Kinetic modelling of the impurity ion component can be performed with the 3D guiding-center orbit tracing code GORILLA (“Geometric Orbit Integration with Local Linearization Approach”) [Eder20, Eder19] that has been recently developed in collaboration of TU Graz / ÖAW and IPP Garching. Being a generalization of the 2D geometric integrator [Kasilov16] used in the 2D kinetic transport code K2D [Runov15] it offers computational efficiency, tolerance to statistical noise in the electromagnetic field and efficient scoring of statistical data. This is achieved by a special piecewise linear representation of the electromagnetic field using a 3D tetrahedral discretization of space which results in a piecewise linear set of the guiding-center equations while retaining the symplectic property of the original set.

- **JINTRAC** is a coupled code package for JET combining 27 physics modules, including 1D transport codes for core plasma transport and edge transport [Romanelli14]. The code package is applied to simulate W transport in a 2D approximation from the source into the pedestal region, and in a 1D approximation from the pedestal to the centre of the core plasma for JET [Koechl17, Casson20] and ITER [Koechl20]. JINTRAC has been used with ad-hoc ELM models to simulate the impact of ELMs of W sputtering and core transport. In this work JINTRAC will be used to interpret JET H-mode plasmas, and to validate its prediction of the W sources (EIRENE), divertor screening (EDGE2D-EIRENE), transport across the separatrix and pedestal and into the core (e.g., QualLiKiz and NEO). Furthermore, the 2D predictions of W transport in the SOL will be compared to 3D predictions using ERO2.0, EIRENE-KIT and EMC3-EIRENE

Key Deliverable 1:

Validated suite of 3D codes and transport models to describe in an integrated way the W content and its distribution in metallic devices, in particular DEMO and ITER, with discrimination of main chamber and divertor sources, screening, transport, and exhaust along with its impact on the main plasma dynamics and performance.

In order to address this key deliverable we have organized the work in three sub-tasks. The first one concerns the code development and verification for SOLEDGE3X, EMC3-EIRENE and ERO2.0. The second one is focused on pedestal studies, with GyselaX and VENUS-LEVIS codes. Finally, the third sub-task is dedicated to the validation step proposing three specific experiments on WEST, W7X and JET tokamaks.

TASK1 for key deliverable 1: numerical development and verification of SOLEDGE3X, EMC3-EIRENE and ERO2.0 codes.

The milestones from M1.1 to M1.11 refer to work related to SOLEDGE3X code while the ones from M1.12 to M1.18 to EMC3-EIRENE (ERO2.0 being connected to both codes)

ID	Milestone-description	participants	Target date
M1.1	Implementation of a 3D wall (i.e. with objects toroidally localized) in SOLEDGE3X-EIRENE	H. Bufferand, Y. Marandet	12/2021
M1.2	Integrating Gorilla orbit tracing code into EIRENE, first step: test of the efficiency of resulting combination in axisymmetric tokamak geometry	M. Eder, Y. Marandet, M. Raghunathan	12/2021
M1.3	Develop interface for importing SOLEDGE3X plasma backgrounds into ERO2.0	H. Bufferand, J. Romazanov	06/2022
M1.4	Review and implement "advanced" sheath BC for multispecies plasma in SOLEDGE3X (in connection with TSVV 3)	H. Bufferand, G. Ciraolo	06/2022
M1.5	Implement complex magnetic geometries into SOLEDGE3X (first with ripple effects)	H. Bufferand, G. Ciraolo	06/2022
M1.6	Integrating Gorilla into Eirene, second step: Implement 3D electromagnetic	M. Eder, Y. Marandet,	12/2022

	field perturbations from the external code, test the accuracy of orbit tracer and optimize the grid for specific perturbations	M. Raghunathan	
M1.7	Integrating Gorilla into Eirene, third step: Implement energy and momentum conserving collision integral for the full-f computations. Generalize this operator for multi-species plasmas with bulk species (main ions and electrons) described externally	M. Eder, Y. Marandet, M. Raghunathan, D. Harting	12/2022
M1.8	Implementation of the EIRENE Kinetic Ion Trace module in SOLEDGE3X	H. Bufferand, Y. Marandet, M. Raghunathan	03/2023
M1.9	Assess sensitivity of BC for multispecies plasma on plasma behavior in SOLEDGE3X	H. Bufferand, G. Ciraolo	06/2023
M1.10	Implementing 3D complex magnetic geometries in SOLEDGE3X (RMP)	H. Bufferand, G.Ciraolo	01/2024
M1.11	Implement (D,v) map for W transport in pedestal region in SOLEDGE3X	H. Bufferand, G. Ciraolo	06/2024
M1.12	Include stabilization scheme [Frereichs2019] in EMC3-EIRENE for dissipative divertor conditions	D. Harting, Postdoc FZJ	12/2021
M1.13	Implementation of EIRENE Kinetic Ion Trace module in EMC3 for low Z impurities	D. Harting, Postdoc FZJ	12/2021
M1.14	Assess applicability of EIRENE-KIT with EMC3 for recycling and sticky impurities (for low Z species)	D. Harting, Postdoc FZJ	06/2022
M1.15	Implementation of EIRENE Kinetic Ion Trace module in EMC3 for high Z impurities	D. Harting, Postdoc FZJ	09/2022
M1.16	Assess feasibility of EIRENE-KIT for high Z species (W, Ar) in 2D and 3D with EMC3	D Harting, Postdoc FZJ	01/2023
M1.17	Demonstrate stable feedback of EIRENE-KIT (radiative cooling) for seeding impurities on EMC3 solution in 2D steady state (closed loop) under semi-detached conditions	D. Harting, J. Romazanov, Postdoc FZJ	06/2023
M1.18	Further verification of EIRENE-KIT on EMC3 plasma backgrounds: comparison with ERO2.0 results (post processing treatment on EMC3 plasma backgrounds)	D. Harting, J. Romazanov, Postdoc FZJ	12/2023

The sub-deliverables proposed as evidence for achieving key deliverable #1 for task 1 are given below

ID	Deliverable-description	Indicator	Participants	Target date
D1.1	Assessment on the Implementation of EIRENE Kinetic Ion Trace module in EMC3 for low Z impurities	Report, paper or presentation	D. Harting, Postdoc FZJ	12/2021
D1.2	Assessment on the Implementation of the EIRENE Kinetic Ion Trace module in SOLEDGE3X	Report, paper or presentation	Y. Marandet, H. Bufferand, M. Raghunathan M. Eder	06/2023
D1.3	Assessment on the applicability of EIRENE-KIT with EMC3 for recycling and sticky impurities	Report, paper or presentation	D. Harting, Postdoc FZJ	12/2023
D1.4	Assessment on the implementation of 3D complex magnetic geometries in SOLEDGE3X (RMP)	Report, paper, conference presentation	H. Bufferand, G. Ciraolo	01/2024
D1.5	Verification of EIRENE-KIT on EMC3 plasma backgrounds: comparison with ERO2.0 results (post processing treatment on EMC3 plasma backgrounds)	Report, paper or presentation	D. Harting, J. Romazanov, Postdoc FZJ	01/2024

Task 2 for key deliverable 1: GyselaX and VENUS-LEVIS code development for investigation for W transport in the pedestal region

ID	Milestone-description	participants	Target date
M1.19	Implementation of a source term in the vorticity equation of Gysela code (following what had been done previously, see A. Strugarek et al., PRL (2013)]:	E. Gravier, PhD student CEA (funded by other means)	12/2021
M1.20	Generation of transport barriers relevant for ITER scenarios with GyselaX code	E. Gravier, PhD student CEA (funded by other means)	12/2022
M1.21	GyselaX simulations with light and heavy impurities	E. Gravier, PhD student CEA (funded by other means)	12/2023
M1.22	Analysis of GyselaX simulations with light and heavy impurity species relevant for ITER (Ne, Ar, W) will be analyzed and compared in nonlinear simulations with and without transport barriers	E. Gravier, PhD student CEA (funded by other means)	06/2024

M1.23	Verification of VENUS-LEVIS against M1.21 for axisymmetric non-rotating ITER/DEMO pedestal (W neoclassical transport),	PhD/Postdoc EPFL, J. Graves	06/2024
M1.24	Derivation of “reduced” models and (D,v) maps for impurities	E. Gravier, PhD student CEA (funded by other means), G. Ciraolo	12/2024
M1.25	Generalisation of M1.23 using VENUS-LEVIS code to include centrifugal effects,	PhD/Postdoc EPFL, J. Graves	12/2024
M1.26	Continuing the investigation with GyselaX simulations expanding the database for reduced models.	E. Gravier, PhD student CEA (funded by other means)	12/2025
M1.27	Generalisation of M1.25 with VENUS-LEVIS code to include 3D equilibria effects (from RMP coils or/and EHOs) and NTV/flows,	PhD/Postdoc EPFL, J Graves	12/2025

The sub-deliverables proposed as evidence for achieving key deliverable #1 for task 2 are given below

ID	**Deliverable-description**	**Indicator**	**Participants**	**Target date**
D1.6	Analysis of results from the generation of transport barriers relevant for ITER scenarios with GyselaX code	report, paper or conference contribution	E. Gravier	06/2023
D1.7	Analysis of GyselaX simulations with light and heavy impurity species relevant for ITER (Ne, Ar, W)	report, paper or conference contribution	E. Gravier	06/2024
D1.8	Derivation of “reduced” models and (D,v) maps for impurities from gyrokinetic simulations (both GyselaX and VENUS-LEVIS)	report, paper or conference contribution	E. Gravier, G. Ciraolo, J Graves, PhD/Postdoc EPFL	12/2024

Task 3 for key deliverable 1: Validation of numerical tools on selected experiments on WEST, W7X and JET

M1.28	SOLEDGE3X 3D plasma background with fluid impurities for WEST experiment in double null configuration	H. Bufferand, G. Ciraolo, Y. Marandet	10/2022

M1.29	ERO2.0 runs on SOLEDGE3X WEST plasma backgrounds and comparison with experimental results	J. Romazanov, G. Ciraolo, Y. Marandet,	01/2023
M1.30	Validation of EIRENE-KIT in EMC3 context on $C^{13}H_4$-tracer experiment at W7-X	D. Harting, Postdoc FZJ, in coordination with W7-X working group	03/2023
M1.31	Execute and validate JINTRAC simulations in JET ELMy H-mode plasmas, characterise dominant transport process leading to core W accumulation, including ELMs	H. Kumpulainen	03/2023
M1.32	W transport validation of EIRENE-KIT on JET for (C30c / M18-18) utilizing horizontal vs. vertical target configurations	D. Harting, H. Kumpulainen	12/2023
M1.33	Contrast 2D JINTRAC against EMC3-EIRENE and SOLEDGE3X predictions to assess 3D effect of W transport	D. Harting, J. Romanzanov, H. Kumpulainen, H. Bufferand, G. Ciraolo	12/2025
M1.34	SOLEDGE3X 3D plasma background with kinetic impurities for WEST experiment in double null configuration and comparison with experiments	H. Bufferand, G.Ciraolo, Y. Marandet, M. Raghunathan	12/2025

The sub-deliverables proposed as evidence for achieving key deliverable #1 for task 3 are given below

ID	**Deliverable-description**	**Indicator**	**Participants**	**Target date**
D1.9	Validation of EIRENE-KIT in EMC3 context on $C^{13}H_4$-tracer experiment at W7-X	report, publication, or conference contribution	D. Harting, Postdoc FZJ, in coordination with W7-X working group	03/2023
D1.10	Validation of 3D simulations with SOLEDGE3X-ERO2.0 for W transport on WEST experiment	report, publication, or conference contribution	G. Ciraolo, H. Bufferand, J. Romazanov	03/2023
D1.11	Comparison of W influx across separatrix based on JINTRAC, EMC3-EIRENE and ERO2.0	report, publication, or conference contribution	Harting, Kumpulainen, Romazanov	12/2023

Key Deliverable 2:

Assessment of the W influx, W screening, and W transport in ITER plasmas envisaged for pre-fusion and fusion power operation with semi-detached divertor and application of resonant magnetic perturbations for ELM suppression. Discussion of the impact on a potential loss of semi-detachment and ELM suppression on the W influx, W screening, and W transport in those ITER scenarios.

ID	Milestone-description	participants	Target date
M2.1	Review and document ITER scenarios to be modelled	All (site activity managers are responsible for local coordination)	06/2021
M2.2	2D Plasma background in semi-detached conditions (no RMP) (both with EMC3-EIRENE and SOLEDGE3X)	D. Harting, H. Bufferand, G. Ciraolo	12/2021
M2.3	Characterization of W transport on 2D ITER plasma backgrounds obtained in M2.2 using ERO2.0 (post processing): discrimination between divertor and main chamber W sources	J. Romazanov, G. Ciraolo	12/2022
M2.4	EMC3-EIRENE ITER plasma background with 3D perturbation in semi-detached conditions (full 3D solution)	D. Harting, Postdoc FZJ	06/2022
M2.5	ERO2.0 runs on 3D ITER plasma backgrounds obtained in M2.4 and characterization of W transport	J. Romazanov	01/2023
M2.6	SOLEDGE3X Plasma background with 3D perturbation in semi-detached conditions: focus on time evolution with semidetached regime which is lost and then recovered	H. Bufferand, G. Ciraolo	06/2023
M2.7	ERO2.0 post processing runs on 3D ITER plasma backgrounds with loss and recover of semidetached condition for characterization of W transport	J. Romazanov, PhD CEA (funded by other means)	12/2023
M2.8	3D production runs for W transport with EMC3-EIRENE and EIRENE-KIT under semidetached divertor conditions with RMP's for ITER: Pre-fusion and fusion power operation in steady state	D. Harting, Postdoc FZJ	12/2024
M2.9	3D production runs for W transport with EMC3-EIRENE and EIRENE-KIT under semidetached divertor conditions with RMP's for ITER: Assess impact on potential loss of semi-detachment (only in steady state)	D. Harting, Postdoc FZJ	12/2025

M2.10	3D production runs for W transport with SOLEDGE3X and ERO2.0: focus on the impact of turbulence on radial transport (using k-eps SOLEDGE3X version)	H. Bufferand, G. Ciraolo, J. Romazanov	12/2025
M2.11	Investigation on W penetration into the pedestal region using (D,v) maps for W obtained from gyrokinetic simulations and implemented into SOLEDGE3X	H. Bufferand, G. Ciraolo, J. Romazanov, E. Gravier	12/2025

The sub-deliverables proposed as evidence for achieving key deliverable #2 are given below

ID	**Deliverable-description**	**Indicator**	**Participants**	**Target date**
D2.1	Characterization of W transport on 2D ITER plasma backgrounds obtained in M2.2 using ERO2.0 (post processing): discrimination between divertor and main chamber W sources	report, paper or conference contribution	J. Romazanov, D. Harting, H. Bufferand, G. Ciraolo, Y. Marandet, PhD CEA (funded by other means)	01/2023
D2.2	Analysis of EMC3-EIRENE ITER plasma background with 3D perturbation in semi-detached conditions (full 3D solution)	report, paper or conference contribution	D. Harting, Postdoc FZJ	12/2022
D2.3	characterization of W transport using ERO2.0 runs on 3D ITER plasma backgrounds obtained in M2.4	report, paper or conference contribution	J. Romazanov	03/2023
D2.4	Analysis of SOLEDGE3X ITER plasma background with 3D perturbation in semi-detached conditions: focus on time evolution with semidetached regime which is lost and then recovered	report, paper or conference contribution	H. Bufferand, G. Ciraolo, Y. Marandet	01/2024
D2.5	Assess impact on potential loss of semi-detachment (only in steady state) using 3D production runs for W transport with EMC3-EIRENE and EIRENE-KIT under semidetached divertor conditions with RMP’s for ITER	report, paper or conference contribution	D. Harting, Postdoc FZJ	12/2025

D2.6	Investigation on W penetration into the pedestal region using (D,v) maps for W obtained from gyrokinetic simulations and implemented into SOLEDGE3X	report, paper or conference contribution	G. Ciraolo, H. Bufferand, E. Gravier, PhD/Postdoc EPFL, J. Graves	12/2025

Key Deliverable 3:
Applications of the developed model. Assessment of the seeding impurity screening and transport in DEMO and ITER scenarios.

ID	**Milestone-description**	**participants**	**Target date**
M3.1	Review and document ITER and DEMO scenarios with seeding impurities to be modelled	All (site activity managers are responsible for local coordination)	06/2021
M3.2	2D ITER Plasma background in semi-detached conditions (no RMP) and N/Ne/… seeding (both with EMC3-EIRENE and SOLEDGE3X with fluid impurities as reference case)	H. Bufferand, G. Ciraolo, D. Harting	06/2022
M3.3	2D ITER Plasma background in semi-detached conditions (no RMP) and N/Ne/… seeding (both with EMC3-EIRENE and SOLEDGE3X with hybrid fluid-kinetic impurities)	H. Bufferand, G. Ciraolo, D. Harting	12/2022
M3.4	3D ITER plasma background with kinetic treatment for seeding low Z species with EMC3-EIRENE	D. Harting, Postdoc FZJ	12/2023
M3.5	3D ITER plasma background with kinetic treatment for seeding high Z species with EMC3-EIRENE	D. Harting, Postdoc FZJ	06/2024
M3.6	3D ITER plasma background with hybrid kinetic-fluid treatment for seeding species with SOLEDGE3X	H. Bufferand, Y. Marandet, G. Ciraolo	06/2024
M3.7	3D productions runs for seeding impurities (Ne, Ar) with EMC3-EIRENE and EIRENE-KIT under semidetached divertor conditions with RMP’s for ITER: Asses screening of seeding impurities (Ne, Ar) due to RMP’s	D. Harting, Postdoc FZJ	12/2025
M3.8	First DEMO simulations (SN configuration) with SOLEDGE3X-ERO2.0 and EMC3-EIRENE	D. Harting, Postdoc FZJ, H. Bufferand, G.Ciraolo, J. Romazanov	12/2025

The sub-deliverables proposed as evidence for achieving key deliverable #3 are given below

ID	Deliverable-description	Indicator	Participants	Target date
D3.1	Analysis of 2D ITER Plasma background in semi-detached conditions (no RMP) and N/Ne/… seeding (both with EMC3-EIRENE and SOLEDGE3X with fluid impurities as reference case)	report, paper or conference contribution	D. Harting, Postdoc FZJ, H. Bufferand, G. Ciraolo, Y. Marandet, M. Raghunathan,	12/2022
D3.2	Analysis of 3D ITER plasma background with kinetic treatment for seeding low Z species with EMC3-EIRENE	report, paper or conference contribution	D. Harting, Postdoc FZJ	12/2023
D3.3	Comparison between 3D ITER plasma background with kinetic treatment for seeding species with EMC3-EIRENE and hybrid fluid-kinetic treatment for seeding species with SOLEDGE3X	report, paper or conference contribution	D. Harting, Postdoc FZJ, H. Bufferand, G. Ciraolo, H. Bufferand	06/2024
D3.4	Analysis of 3D productions runs for seeding impurities (Ne, Ar) with EMC3-EIRENE and EIRENE-KIT under semidetached divertor conditions with RMP’s for ITER: Asses screening of seeding impurities (Ne, Ar) due to RMP’s	report, paper or conference contribution	D. Harting, Postdoc FZJ	12/2025
D3.5	Analysis of First DEMO simulations (SN configuration) with SOLEDGE3X-ERO2.0 and EMC3-EIRENE	report, paper or conference contribution	G.Ciraolo, D. Harting, Postdoc FZJ, H. Bufferand, J. Romazanov	12/2025

Risk assessment

The major risks and mitigation strategies linked to this proposal are summarized in the following table

risk description	Probability	action
Unavailability of computational resources – 3D ITER and DEMO simulations are computationally extremely demanding	moderate	Ask EUROfusion to secure the necessary High Performance Computing resources.

Manpower not available (all tasks) ➔ delay or deliverable not achieved	Low	Ask Research Units to secure/replace the staff members
Unavailability of well-diagnosed experimental inputs for all scenarios in the validation task: ➔ delay or deliverable not achieved	Moderate	Connection with experimental teams has to be renforced with identification of further discharges and if needed requests for new shots have t be submitted
Difficulties (numerical issues and or performances in time computation) with the Kinetic Ion trace module of EIRENE for kinetic treatment of heavy impurities	Moderate	This issue has been extensively discussed between the members of the consortium. Alternatives have been already identified, like the use of ERO2.0 fully coupled to plasma solver. A first assessment at the end of the first year is planned

Expected High Performance Computing requirements

Expected usage of the MARCONI-Fusion supercomputer in the early phase of the project?

- *Anticipated total amount of node hours needed*
- *Anticipated number of nodes required (which partition?)*
- *Special requirements (optional)*

The total amount of node hours required for the compute-intense parts of this project are estimated at about 1 Mnode-hours per year (for the first three years then 1.2 Mnode-hours). Here, the following detailed numbers are considered:

- CEA:
  a) GYSELAX: 0.4-0.5 Mnode-hours on Marconi standard partition per year (avg. 128 nodes)
  b) SOLEDGE3X: 0.150 Mnode-hours, on Marconi standard partition per year (avg. 20 nodes)
- FZJ:
  a) EMC3-EIRENE: 0.3 Mnode-hours on Marconi standard partition per year (64 nodes)
  b) ERO2.0: 40 k node-hours on Marconi standard partition per year (256 nodes)
- EPFL:
  a) VENUS-LEVIS: 0.2 Mnode-hours on Marconi standard partition per year (avg. 128 nodes), (starting from 2024)
- Graz TU:
  a) Gorilla simulations : 0.2 knode-hours on Marconi standard partition per year (avg. 20 nodes)

These estimations come from the present experience for the different codes. As an example, we detail here the number of hours necessary for GyselaX computations, which are the most elevated in this request:

GyselaX requirements: 25 million core.hours will be requested per year to perform GYSELA simulations (Marconi). Typical simulations involve meshes with billions of grid points and thousands of time steps. A detailed description of the model equations, numerical methods, and parallelization is available [V. Grandgirard *et al.*, Comput. Phys. Communications, 207, 35 (2016)]). To summarize, parallelization is multi-level, MPI/OpenMP, combining distributed memory and shared memory programming. It was recently optimized for highly multi-threaded environment, with efficient exploitation of SIMD vector units and memory access pattern, leading to a speedup of 3x on Skylake and KNL [G. Latu *et al.*, hal-01719208, (2018)]. The mesh is 5D, with 3 dimensions in real space (radius r, poloidal angle θ, and toroidal angle ϕ), and 2 dimensions in velocity space (parallel velocity v// and magnetic moment μ). The mesh size in real space is determined by the scales of turbulent fluctuations (~mm) and the size of the device (~m). The mesh size in velocity space is determined by previous convergence tests. The number of time steps is determined by the autocorrelation time of turbulence (~ms) and the confinement time (~s). Finally, a typical GYSELA simulation with impurities requires ~10^{11} grid points, and ~10^{4} time steps. Memory requirements indicate a minimum of 24 Marconi-A3 nodes per run.

Expected long-term requirements of HPC resources?

On longer time-scale the numerical requirements are likely to increase at least by a factor of 1.5 as more and more physics will be embedded in the high-level simulations for ITER and DEMO.

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

The Advanced Computing Hubs will cover the following topics and activities:

- *High Performance Computing (scalable algorithms, code parallelization and performance optimization, code refactoring, GPU-enabling etc.)*
- *Integrated Modelling and Control (code adaptation to IMAS, IMAS framework development, code integration etc.)*
- *Data Management (open access, data management, data analysis tools, aspects of AI and VVUQ etc.)*

For further details, please refer to the respective ongoing call, Ref. PMU/1740.

ACH support will strongly contribute to the achievement of our targets. The following list summarizes the expected activities and resources:

1) Concerning **High Performance Computing** the following activities will need strong support
    a) 0.5 ppy on profiling and optimisation of SOLEDGE3X in the case of high number of species (from 2021 to 2025)
2) Concerning **IMAS** aspects:
    a) 0.5 ppy on code adaptation to IMAS (SOLEDGE3X, EMC3-EIRENE, ERO2.0, etc..), focusing firstly on IMAS compatible outputs.

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