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

Title (c.f. Annex-2)	*TSVV Task 5: Neutral Gas Dynamics in the Edge*
TSVV Task leader (name/e-mail)	*Dr. Dmitriy V. Borodin* *d.borodin@fz-juelich.de*
Lead beneficiary	*FZJ (Germany)*
Project duration	*5 + 2 years*

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In addition, several vacancies are suggested (for details see 2 next sections including table 1).

Relevant skills and experiences of the TSVV Task team

Dr. Dmitriy V. Borodin
is a senior researcher at the Institute for Climate and Energy Research – Plasma Physics (IEK-4) in the Research Centre Jülich, Germany. He has 20-year experience in modelling of fusion-relevant plasmas with particular focus on atomic and molecular processes and plasma-wall interaction, SOL and divertor plasmas. D.Borodin has participated in multiple experiments at both tokamaks and linear devices including their coordination as well as modelling-based interpretation of diagnostic observations often with extrapolation of key results for ITER. He has also a relevant experience of organizational work for international research projects including 3-year experience of deputy task force leader for JET-ILW experimental campaigns and decade-long membership in the steering committee of ADAS (Atomic Data and Analysis Structure) consortium. Since 01.01.2020 D.Borodin has stepped in as a leader into the pilot TSVV "neutral gas module" project.

New PhD-student(s) and postdoc for atomic and molecular data (5+2 years in total, depending on the project extension)
A PhD-student is to be hired who's work may be continued by him/herself as a postdoc or by a second student covering altogether up to 7 years of the necessary work. He/she must have good programming as well as data processing and visualisation experience together with strong background in math (including nonlinear dynamics) and elementary processes in plasma including molecular reactions. Expertise and experience in plasma spectroscopy are beneficial.

New computer and IT engineer
is to be hired. He/she must have good programming and data processing experience including web-interfaces, code versioning, data consistency checks and CI. Good experience working with databases, data processing, visualisation are desirable as the engineer is supposed to extend and improve the data infrastructure inherited from EIRENE: AMJUEL, H2vibr, ADAS, etc. Significant part of the job is to maintain and develop further soft- and hardware IT infrastructure necessary for running EIRENE code and its support tools including web-based ones. Code and features documentation is also part of the work package. During initial phase Mrs. Petra Börner (FZJ), who has done EIRENE maintenance for decades, can provide some useful support and advice.

Dr. ir. Wouter Dekeyser
is a permanent researcher at the Department of Mechanical Engineering of the KU Leuven. As a mechanical engineer, he has expertise in computational fluid dynamics (CFD), numerical methods, and numerical optimization for partial differential equations (PDEs), with over 10 years of experience in plasma edge modelling and SOLPS(-ITER) code development. He was involved in several EUROfusion WPCD, ENR and TSVV projects focusing on algorithms for code speed-up, fluid and hybrid fluid-kinetic neutral modelling, and adjoint-based optimization techniques for nuclear fusion divertors.

Prof. dr. ir. Giovanni Samaey
is a research professor in mathematical engineering at the department of Computer Science (KU Leuven). His main expertise is on the development of computational multiscale methods for stochastic particle systems, including time integration, Markov chain Monte Carlo methods and data assimilation, and their implementation in HPC software. The methods he studies find application in plasma edge simulations: he was involved in the EUROfusion Enabling Research project WP14-ER-01-FZJ-03 “Towards enabling computational divertor design for fusion power plant divertors: state of the art adjoint based edge plasma simulation techniques” and co-PI of the project “Adjoint-based optimization methods with fluid/kinetic plasma edge codes for nuclear fusion reactors” with the Research Foundation – Flanders (FWO). G. Samaey was also PI of four PhD students focusing on Monte Carlo estimators and code coupling techniques; and co-PI of two PhD students on hybrid methods and accuracy assessment.

Ir. Bert Mortier
will be a postdoctoral researcher at the Department of Computer Science of the KU Leuven (PhD defence is planned in November 2020). As a mathematical engineer, he has expertise in numerical methods and algorithmic design. During his PhD, he worked specifically on algorithmic improvements for the neutral particle tracing scheme used in the EIRENE code. The currently used particle tracing methods are extensively analysed and a new, asymptotic-preserving Monte Carlo simulation method and accompanying multilevel extension and estimator are proposed, that provide significant speed-up in highly collisional regimes (HCR). This fundamental algorithmic research contributed to the EUROfusion TSVV project “Neutral Gas Module”. He also contributed to a project of the Research Foundation Flanders (FWO) focusing on hybrid fluid-kinetic methods.

Dr. 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 Soledge2D and TOKAM3X). He was involved in the EUROfusion Enabling Research project WP14-ER-01-FZJ-03, “Towards enabling computational divertor design for fusion power plant divertors: state of the art adjoint based edge plasma simulation techniques” and in several other Enabling Research projects.

Ir. Paul Genesio
is a CNRS research engineer at the PIIM laboratory, Aix-Marseille. He has a long-standing experience in code development, parallelization and maintenance. He will also provide direct support for some of the algorithmic aspects (lean code, domain decomposition, OpenMP parallelization including related code refactoring).

Dr. Egbert Westerhof
is currently Theme Leader ad-interim for Fusion Energy and Group Leader for Integrated Modelling and MHD at DIFFER. He has thirty plus years' experience in integrated tokamak modelling with a focus on electron cyclotron heating and current drive and the control of MHD instabilities. In recent years, the scope of his research has broadened to include the study of SOL and divertor plasma. He is a user of the SOLPS-ITER code and develops reduced, control oriented models of divertor detachment.

Dr. Jorge Gonzalez
is a postdoctoral researcher at DIFFER in the Integrated Modelling and MHD group. He earns his PhD in Aerospace Engineering at the Technical University of Madrid developing numerical methods to describe weakly ionized plasmas in interaction with metallic walls and also plasmas applied to space propulsion. He is currently working in the refactoring of EIRENE as well as implementing new features in the code, related with output format, non-analogue scheme and the modelling of Lithium walls.

Prof. Dr. Mathias Groth
is a professor in fusion and nuclear engineering at the Department of Applied Science of Aalto University, Espoo. Finland. His primary expertise is in experimental plasma edge physics and edge modelling. His recent work focused on investigating the role of molecules and photons in detached divertor conditions in JET and DIII-D. His expertise includes the edge fluid codes SOLPS and EDGE2D-EIRENE, as well as EIRENE. He will provide experimental data from dedicated JET experiments to validate neutral models, and perform SOLPS-ITER, EDGE2D-EIRENE and standalone EIRENE simulations to support the task. He is the PhD thesis supervisor of M.Sc. Andreas Holm.

M.Sc. Andreas Holm
is a PhD student at Aalto University, Espoo, Finland, studying the impact of molecules on detachment using fluid (UEDGE), coupled fluid-kinetic (EDGE2D-EIRENE) and neutral Monte-Carlo (EIRENE, DEGAS2) codes. As part of his Fulbright scholarship, carried out at Lawrence Livermore National Laboratory in 2019-20, he implemented the Greenland 2000 collisional-radiative model for atoms and molecules in UEDGE. His primary contribution to the project will be implementing atomic and molecular rates and collisional-radiative models for deuterium and tritium in the neutral gas code. He will be comparing the predictions from the neutral gas code to those from the present EIRENE in simple simulation geometries, and to experimental data from JET.

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

The expected commitment is given in the following table. It should be noted, that the particular persons may change in future, in particular non-permanent staff like PhD-students. However, the distribution of the workload between the RUs should remain roughly the same throughout the time frame, with the main expected change being a shift of focus from algorithmic improvement in 2021-2023 – with support from the ACH IM and liaison prof. G. Samaey (KUL) towards validation in 2024-2027 with guidance and valuable experience from prof. M.Groth (Aalto University).

Table 1. *Expected commitments from the participants and research units (RUs); CP is "contact person for a RU".*

Participant			Commitments, in person-months (PM)						
Name	**RU**	**Role in TSVV-5**	**2021**	**2022**	**2023**	**2024**	**2025**	**2026**	**2027**
Wouter Dekeyser	KUL	**CP KUL, senior scientist,** fluid-kinetic hybridisation, adjoint approach, time-dependent runs, predictive case for DEMO	6	6	6	6	6	6	6
Bert Mortier	KUL	**Postdoc**, fluid-kinetic hybridisation, adjoint approach, predictive case for DEMO	9	9	9	9	9	9	9
Giovanni Samaey	KUL	**Senior scientist**, **consultant (partially covered by other means)**, algorithmic development, liason to ACH IM	3	2	2	0	0	0	0
Dmitriy Borodin	FZJ	**Task Leader, CP FZJ, senior scientist**, CRMs for molecules, AMNS, detachment, EIRENE as NGM: code development, validation and maintenance	9	9	9	9	9	9	9
Vacancy	FZJ	**Computer and IT engineer**, EIRENE as NGM: code development, validation and maintenance, support of AMNS database and web-services	6	6	6	6	6	6	6
Vacancy	FZJ	**PhD-student or postdoc**, CRMs for molecules, AMNS database structure and content, detachment	9	9	9	9	9	9	9
Egbert Westerhof	DIFFER	**CP DIFFER, consultant (fully covered by other means),** senior scientist, FE model for the divertor targets and FW, code applications to MAGNUM-PSI experiments	0	0	0	0	0	0	0
Jorge Gonzalez Munoz	DIFFER	**Postdoc**, FE model for the divertor targets and FW, Validation by applications to MAGNUM-PSI	6	6	6	none	none	none	none
Vacancy	DIFFER	**Same as above**	none	none	none	6	6	6	6
Yannick Marandet	CEA	**CP CEA, senior scientist,** EIRENE expert, domain decomposition, algorithm for time dependant mode, modularisation, HPC	6	6	6	6	6	6	6
Paul Genesio	CEA	**Computer Engineer,** Parallelization, modularisation of the code	6	6	6	6	6	6	6
Mathias Groth	Aalto Univ.	**CP Aalto, senior scientist, consultant (partially covered by other means)**, validation at JET and predictions for ITER, detachment, CRMs for atoms and molecules	0	0	0	3	2	3	2
Andreas Holm	Aalto Univ.	**PhD-student, later postdoc** fluid-kinetic hybridisation, EIRENE as NGM: code development for HPC	9	10	10	9	10	9	10
	ACH IM	Algorithmic improvement	6	6	6	6	6	6	6
	ACH HPC	Parallelisation	6	6	6	6	6	6	6

	ACH D, IM	AMNS, catalogued simulations	3	3	3	3	3	3	3
PM (total)			**84**	**84**	**84**	**84**	**84**	**84**	**84**
PPY (total)			**7**	**7**	**7**	**7**	**7**	**7**	**7**
ACH/total			17,86%	17,86%	17,86%	17,86%	17,86%	17,86%	17,86%
			2021	**2022**	**2023**	**2024**	**2025**	**2026**	**2027**

Short description (as in the IMS)

Neutral gas physics and its interactions with the plasma is a key aspect of edge plasma and divertor physics in a fusion reactor. The proposal foresees the development, verification and validation of a Neutral Gas Module (NGM) based on the existing EIRENE code to establish a flexible, efficient and reliable computational tool. The NGM will provide efficient use of high-performance computing (HPC) resources including domain decomposition and demonstration of good speedup scaling for hybrid OpenMP-MPI parallelisation in a view of significant volumes and numbers of traced Monte-Carlo particles. The NGM will be employable in any 2D or 3D integrated modelling approach for simulation of fusion reactor regimes with (semi)detached divertor on ITER and DEMO scale. The interfaces to other codes will be adopted for IMAS (Integrated Modelling and Analysis Suite platform) and liaised with other TSVVs, in particular, TSVV-3&4.

The physics improvements will include refined and extended collisional-radiative models (CRMs) for molecules including resolving the rotational and vibrational states, adding reactions types (e.g. for photon absorption) and treatment of isotope effects for H_2, D_2, T_2, DT and molecular ions. A significant focus will be given to building a hierarchy of models including advanced fluid neutrals and various fluid-kinetic hybridisations (FKH), which are to approach the accuracy of the full-kinetic runs, while providing an efficient treatment of highly collisional regions (HCR). These models will enable efficient simulations for ITER and DEMO.

The proposal includes significant modernisation of the EIRENE basic structure: modulisation will allow segregating the numeric core from all branching, data pre-processing and interfaces; new models and features will be provided, including a finite element model (FEM) for the divertor target (W) and its proxy at MAGMUM-PSI (the FEM will also be able to treat first wall (FW) elements); modifications providing time-dependent simulations and the use of the adjoint approach for sensitivity studies and uncertainty quantification (UQ) are foreseen. The proposed NGM infrastructure conform with up-to-date standards includes version control, continuous integration and repository for the simulated data for the selected simulation base cases.

The proposal contains a strong validation part with experiments at JET-ILW, MAGNUM-PSI and PSI-2. Predictive power and computational performance will be demonstrated for ITER (focus on semi-detached divertor scenario) and DEMO (focus on usability and advantages of FKH for HCR). The validation effort will be focused on detachment physics including improved CRMs and photon trapping (spectroscopy for well-characterised plasma conditions) as well as on testing of improved coupling to plasma-surface interaction physics including transients utilizing the target/FW FEM.

Motivation, work scope and document organization

Neutral gas physics and its interactions with the plasma is a key aspect of edge plasma and divertor physics in a fusion reactor. A full physics description of the neutral gas dynamics requires a 6D kinetic approach, potentially time dependent, where the details of the wall geometry play a substantial role, to the extent that, e.g., the subdivertor region has to be included. Furthermore, the models involve multiple species, e.g., in a mixed D-T plasma there are 3 different types of molecules, for which each vibrational and even rotational state may have to be tracked. The Monte-Carlo (MC) approach used in EIRENE [1], is in our view best suited to solve these types of complex problems.

30 years of experience are embedded into EIRENE, including coupling to current computational fluid dynamics (CFD) edge codes (e.g., the well-established SOLPS package in which B2.5 and EIRENE are iteratively solved and applied to 2D poloidal tokamak grids). It is essential to build on this expertise and advanced the computational methods. Nonetheless, it is also important to derive a hierarchy of models by accuracy and clearly identify for what type of physics issue they provide reliable answers. In the pilot phase of the TSVV project, we have demonstrated that advanced fluid neutral (AFN) models are very accurate in high-collisional regimes (HCR), and at least an order of magnitude faster than fully kinetic simulations. By including a separate neutral energy equation, their range of applicability has also been extended towards lower collisionalities [2]. Moreover, the use of advanced boundary conditions, based on numerical integration of table data (from SDTrimSP code) for plasma-wall interaction (PWI) allows capturing the effects of varying wall materials (e.g., C, W, Be) on recycling properties, aspects that are currently only crudely – if at all – included in previously existing fluid neutral models. Finally, an initial study has demonstrated that the models retain their efficiency when coupled with kinetic molecules. The AFN models also form the basis of fluid-kinetic hybrid (FKH) models, which combine the accuracy of fully kinetic simulations with the speed-up of fluid neutral models. Such methods were originally developed in the context of radiation transport [3], and later on also for neutron transport [4] and the Boltzmann-BGK equation [5]. Three approaches are introduced: a spatially hybrid technique (SpH), a micro-Macro hybrid method (mMH), and an asymptotic-preserving Monte-Carlo (APMC) scheme. However, mostly these developments are currently at a "proof of principle" stage, thus not yet routinely applied to tokamak scales and realistic geometries.

The proposal foresees the development, verification and validation of a Neutral Gas Module (***fig. 1***) based on the existing EIRENE code. It will become a flexible and reliable tool, both in terms of performance/stability as well as in terms of physics and underlying data, employable in any (2D or 3D) integrated modelling approach for simulation of fusion reactor regimes with (semi)detached divertor on ITER/DEMO scale.

In accordance with the aims of the project stated in the call, we will

- evolve the EIRENE code towards a **modern optimized HPC Monte-Carlo (MC) solver** with more versatile parallelisation schemes aimed at reducing the memory footprint for large grids suitable for 2D and 3D ITER/DEMO scale simulations. The EIRENE internal structure should be re-thought including segregating the compact numeric core and providing domain decomposition.
- improve the coupling schemes to other codes for HPC and adopt those to Integrated Modelling and Analysis Suite (IMAS), to **turn EIRENE into a "neutral gas module" (NGM) efficiently adaptable to other TSVV codes** including in direct coupling schemes. The proposal includes liaising with other TSVVs (in particular, TSVV-3&4) to ensure the full hierarchy of models listed in the next bullet can be used once these other new tools become mature.
- develop and qualify fluid (incl. AFN) and hybrid kinetic/fluid descriptions to **provide a multi-fidelity hierarchy of models**. The model limitations and advantages will be studied to select an optimal (combination of) scheme(s) to be employed in the NGM. Numerical issues will be addressed and improved algorithms and control parameters provided.
- revisit and **extend the Atomic and Molecular data and collisional-radiative models** (CRMs): introduce ro-vibrational temperature as parameter, provide data for H/D/T isotopes and photon tracing, (PWI) data including extension to the reduced models covering in a heuristic way the processes like FW outgoing and recycling including the role of the isotopes, chemically-assisted physical sputtering (CAPS), etc.
- **establish a portfolio of interconnected cases** for testing, validation (main focus on JET-ILW and MAGNUM-PSI) and prediction (ITER) that facilitate testing of particular models/improvements as

well as assessing total predictive power of EIRENE as NGM. These applications are also supposed to demonstrate sufficient numerical performance on ITER and DEMO scales reached both by efficient HPC utilization as well as due to FKH.

- **apply NGM to simulations of well-diagnosed, detached JET-ILW, MAGNUM-PSI and PSI-2 plasmas** to elucidate the impact of ro-vibrationally excited molecules on the onset and degree of detachment (molecular assisted dissociation, recombination, ionisation), develop synthetic diagnostics in NGM and validate predictions against molecular spectroscopy, assess impact of isotope species on detachment.
- **develop photon tracing module in NGM**, evaluate degree of Lyman photon opacity and assess effect on degree of detachment.
- **provide a generic coupling of the NGM-CFD code with a Finite Element Model for the divertor** target (W). Validation with MAGNUM-PSI experimental runs with a focus on wall temperature and detachment conditions in time-dependent runs for transients.
- **expand JET and MAGNUM-PSI analyses to ITER-like plasma and neutral conditions, upscale the geometry and volume**, including ro-vibrationally excited molecules and Lyman photon opacity, (semi)detachment, impact of the divertor target conditions, etc. Evaluate relevance of included processes.

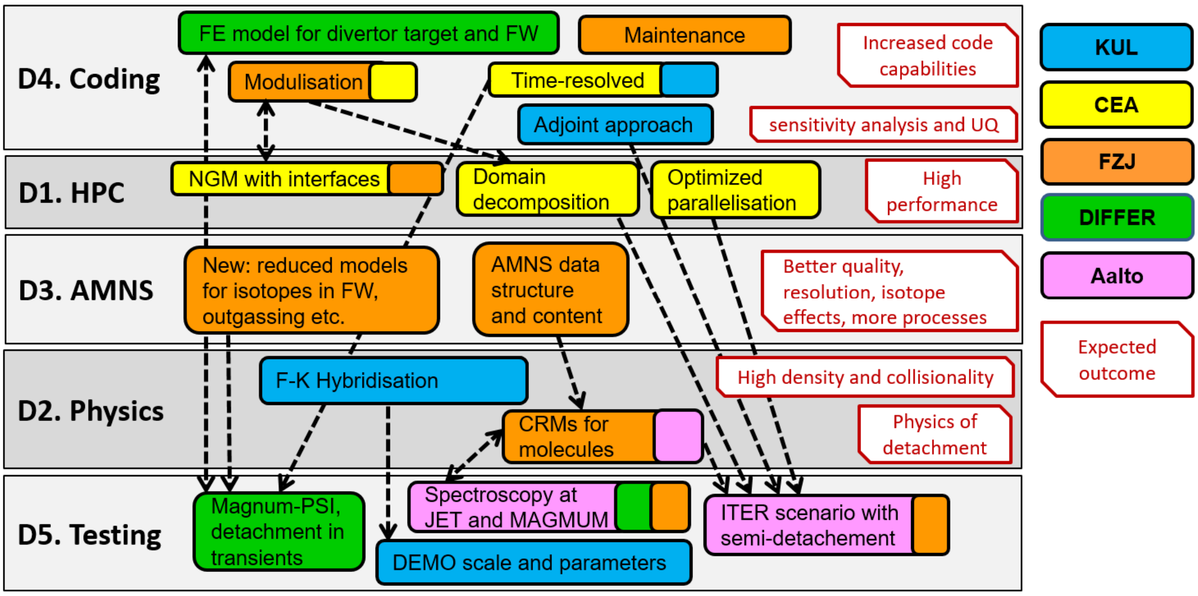


Figure 1. *General view of the subtasks in TSVV-5, grouped by the call deliverables D1-D5 and most important interconnections; RU contributions are colour-coded.*

The document is organized as follows. The workplan (next section) is structured by the top deliverables ***D1-D5*** as they are given in the call. We have developed a list of SMART deliverables "***DN.a***", "***DN.b***", etc. which are also summarized in the ***table 2*** with more details: subtasks, milestones and risks including dependencies. The list of participants and their roles is given in ***table 1***. A very general scheme of the project scope is given in ***fig.1***. The suggested timeline for 2021-2027 (somewhat simplified for readability) is given in ***fig.2***.

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

Detailed work plan with specific deliverables (D1-D5 are as in the call):

D1. Neutral gas code that allows for an efficient use of HPC resources (towards exascale systems and/or HPC booster techniques) through suitable parallelization methods.

a. ***Lean MC code for HPC applications including interfaces to TSVV-3,4,6 etc.*** This work will benefit from the general restructuring of the code carried out for ***D4.c*** and ***D4.d***, which will eliminate all unnecessary branching for a given case and enable optimization of the core MC calculation for each relevant geometry (grid type) option. The algorithms used to calculate intersections with the grid cells boundaries are critical for code performance and will be further optimised. This work will benefit from code profiling with the support of an HPC ACH. The potential of sparse storing schemes will be investigated for output tallies. The optimisation of the parallelisation is a major aspect and is dealt with in ***D1.b*** and ***c***. Another important aspect is the optimisation of the interface to fluid codes, which should provide plasma conditions to the core solver. The latter (set of cell parameters for a volume grid) have to be pre-processed in cases with complex chemistry and/or when collisional radiative models have to be used, as the computation of rate coefficients in every cell can lead to a substantial overhead. We will rewrite the EIRENE code such that coupling to other codes is done via well-defined interfaces, fully conforming with the HPC demands. The segregated from the numeric core "starter" part (executed once per simulation case) developed in ***D4.c*** (handling input files and pre-processing to set-up sandbox-like environment for the core free of case-specific details) should provide inheritance of the former functionality of EIRENE and extend it. In case of a coupled run (e.g. to CFD code), part for the starter job will be setting up the interface based on the standard framework adopted for IMAS. We will develop a transparent, intuitive and well-documented workflow (including necessary scripts, wrappers and other support codes), first on example of NGM coupling to fluid codes (in cooperation with TSVV-3, in particular with respect to the coupling scheme) and later in a fully general way. The same standard interface will be used for coupling with the FE target model in ***D4.b***.

b. ***Domain decomposition.*** The parallelization of the linear Monte-Carlo scheme used by EIRENE is conceptually simple, and EIRENE was initially parallelized with applications requiring a massive number of particles in mind, using MPI. However, with large 3D grids (up to typically ~10^9 grid cells in future applications for a reactor class machine with Larmor radius resolution) with ~100 fields to store, memory poses a limitation at the node level. This can be addressed to some extent by adding a shared memory layer, following the successful OpenMP parallelization layer implemented during the pilot phase. However, the communication overhead needed to transfer the full grid to computation nodes can become significant, and ultimately the full grid will simply not fit on a single node. As a result, a domain decomposition strategy will be pursued, since the later has strong potential for large cases and should also provide additional flexibility for core/thread load balancing. The shared parallelization layer can still be used at the node level, on a chunk of the grid, or even offloaded to a booster/GPU unit. This work will require addressing several inter-related issues, like grid partionning, communication handling, load balancing. The positive experience of other communities for similar problems will be reviewed and exploited. Some guidance and support from ACH HPC will be useful.

c. ***Parallelisation optimisation.*** The performance of the parallelization implemented during the pilot phase remains to be fully assessed and optimized. This work is ongoing at the time of writing with the help from high level support team (HLST). The constraints related to an efficient parallelization of the particle loop will be properly taken into account in the refactoring process of the code. We will address the scoring of trajectories into shared tally arrays, which is a key hotspot. Shared memory parallelization of the starter phase will also be implemented where needed, e.g., in cases where a CR model has to be run in every cells. Optimisation of the implementation of the domain decomposition scheme (***D1.b***), through MPI, will be done subsequently. We will also design global optimal load balancing strategies, taking advantage of the two OpenMP and MPI parallelization layers. These activities will be carried out with the support of an HPC ACH.

D2. Revised and extended physics basis for the neutral gas model. Further development of the underlying collision-radiative model towards the full vibrational resolution for all hydrogen isotopes and specific impurities for seeding.

a. ***Spatial FKH***. We will develop spatially hybrid FKH schemes to extend the feasibility of kinetic simulations to more complicated physical situations. The SpH method [6], [7] is conceptually the most direct method. It combines a fluid model in regions of high collisionality (e.g. divertor), with a kinetic model in less collisional regions (e.g. upstream), using appropriate interface conditions. In this task, we will further develop the fluid neutral models that form the basis of the hybrid methods. Important effects such as plasma drifts, neutral-neutral collisions, and multi-species plasmas (specifically mixed H/D/T plasmas) need to be included. The resulting models can serve as a basis for the ones needed by drift-fluid, gyro-fluid and possibly gyro-kinetic codes in the related TSVVs 3 and 4. Second, the interface conditions are at present subject to judgement of the modeller, and as such prone to modelling error. We will further optimize the performance of the coupling to molecules. Finally, while the current hybrid methods have only used fluid models for the atoms, we will investigate whether fluid and hybrid models for the molecules can be derived, to further speed up the overall simulation.

b. ***FKH as kinetics-based correction***. An alternative hybrid approach is the mMH hybrid method [8], which combines a fluid model with a kinetic correction in the entire simulation domain. This approach is very promising because it incurs, at least in principle, no modelling error compared to a fully kinetic neutral simulation. However, at present some simplifying assumptions regarding the fluid neutral distribution are made in the fluid-kinetic interface to facility the sampling of kinetic correction particles, which lead to a modelling error in the current implementation. We will use rejection sampling to reduce these modelling errors in the mMH method. Second, while the mMH technique already achieved a speed-up of up to a factor 5 compared to kinetic simulations, the main remaining bottleneck for the performance of the mMH method stems from large bias and cancellation errors originating from the presence of positive and negative kinetic correction particles. We will further develop the mMH method to reduce these cancellation errors and enhance its performance further. Third, a different set of hybrid approaches are the so-called asymptotic-preserving. Monte Carlo (APMC) methods [9]. These methods use a single particle scheme throughout the entire domain, in such a way that the method automatically obtains the accuracy of a standard Monte Carlo simulation in the low-collision regions, and the efficiency of a random walk simulation in the high-collision regions. The advantage compared to mMH methods is that no additional grid is required for the fluid approximation. One such method, developed at KU Leuven, is the Kinetic-Diffusion (KDMC) [10]. This method uses hybridized particles that are simulated with a combination of a standard MC procedure with a random walk procedure, which can be considered as aggregating a large amount of collisions without the need for explicitly simulating each individual collision. While the KD scheme is very accurate and efficient both in high- and low-collisional regimes, it suffers from a bias in intermediate regimes. This bias can be eliminated by embedding the method into a multilevel MC framework. Additionally, using the KDMC scheme requires modifications to the track-length procedures to estimate source terms. Appropriate estimators for mass and momentum transport, as devised in [11] in a simplified setting, will be generalized for application in EIRENE. The computational speed-up provided by the FKH methods is expected to enable the efficient simulation of high-collisional ITER/DEMO scenarios, and will be assessed using a series of test cases in ***D5.c***.

c. **Improved CRMs for molecular species and photon tracing.** Atomic and molecular processes in plasma critically determine the trajectory and lifetime of a neutral particle in a plasma: dissociation, ionisation and recombination processes determine the composition of the plasma, elastic and inelastic collisions lead to changes in the trajectory of the particles, and to changes of plasma momentum and energy content. Spectroscopy provides most valuable and extensive, time-resolved measurements for validation (see ***D5***) of the neutral gas module. The models will be tested in simple slab geometries for plasma conditions pertaining to MAGNUM-PSI, JET and ITER. Previous experiments showed that the internal state of the hydrogen molecule, including their rotational and vibrational states, affects the degree of dissociation, ionisation and contribution of molecular-assisted recombination (MAR), which play a key role key in detachment [12] [13]. Thus, ro-vibrational temperature will be introduced as a model parameter. The refined and extended models will be verified against the original collisional-radiative models (CRM) [14] of EIRENE, and, if needed, further developed. In a view of T and DT campaigns at JET [15], ITER and DEMO the isotope effect for hydrogenic species including D and DT will be assessed and implemented. In case ITER decides to select N2 seeding for detachment control, the same resolution will be needed also for N-containing molecules [16]. Recently massive calculations by ab initio methods for basic data are available and ADAS [17] is providing a framework for pre-processing of those rates (see ***D3.a***). A significant part of the CRM development will be validation with spectroscopy experiments at JET-ILW, MAGNUM and PSI-2 [18] in ***D5.a***. The validation process will require iteration of the CRM and underlying data (***D3.b***) development.

D3. Improved (in contents and structure) Atomic and Molecular database for volumetric and surface processes. Database access through generalized interfaces to, e.g., atomic, molecular, nuclear and surface (AMNS) physics data.

a. ***AMNS structure.*** The atomic, molecular and surface data (partially for deuterium and tritium, thus considered nuclear) are an essential part of the NGM package to be developed and refined. They are indispensable for kinetic simulations of plasma particles, which also involve PWI. The structure of these data reflects its physical basis and level of approximation. The structure determines the usability of multiple data sets in the code, including the resulting performance as well as flexibility allowing use of the data with various resolution and quality, which are often limited by the availability of quantum atomic/molecular calculations. ADAS [17] has provided recently new "mdf" data formats systematically organizing the pre-processing and use of the molecular data similarly to the "adf" formats already successfully used for decades including by the EIRENE code [1]. We will use data such as [19], which is planned to be available in ADAS soon, or will assemble and convert other necessary data from literature [20] or collaborators into the same format and utilize as a basis for our improved CRMs (***D4.c***). We will develop data processing and analysis tools within EIRENE-NGM as well stand-alone. The recycling and outgassing from the wall as well as divertor plates and FW erosion (PWI) for plasmas with multiple species (H/D/T, D_2, D_2^+, DT, …) is critical for divertor physics. This issue can, however, be addressed on realistic timescales on the basis of reduced models with fitted parameters. The related data will be introduced into the NGM database, which puts special demands on its flexibility and variability as well as good logging and documentation.

b. ***AMNS content.*** The content of the database requires extension and refinement, for example, for instance for ***D4.c*** we will include into it ro-vibrationally resolved rates for hydrogenic and other critical for the reactor molecules in (e.g. N-family in case N_2 seeding will be used ITER). The large collection of the PSI data (sputtering, reflection, etc) will be revisited as the main production tools like the SDTrimSP code have been significantly improved over the last decade. In addition, new sources of data have become available just very recently (e.g. massive R-matrix [19] *ab initio* simulations of molecular data, which were limited earlier due to performance issues even for moderately complex atoms). At last the validation, in particular in ***D5.a*** (A&M), ***D5.b*** (PSI) is likely to reveal some gaps or inconsistences in the data. The task is to select carefully from the sources and to incorporate into the database the best available data. Taking into account the foreseeable increase in the data variability, amount and complexity, part of the task will be establishing routine procedures and developing automatic conversion, consistency checks and logging tools. We also plan to introduce and index of the data used in the predictive and validation runs (at least across our portfolio cases), which should help in assessment of any particular data set: its quality, impact on simulation results, resolution, consistency etc. It will also help to identify the simulations, which need recalculation in case any data issues are revealed. We propose additional improvement by unification and cross-check of the database with the codes employed for close or even partially intersecting purposes e.g. B2 or ERO utilized in TSVV-3 and TSVV-6,7 respectively.

D4. Interfaces and boundary conditions necessary for future applications; modularization of the neutral gas code to facilitate coupling to computation fluid dynamics (CFD) codes (2D or 3D codes, turbulence codes, time-dependent) and possibly also to gyro-kinetic/gyrofluid plasma codes.

a. ***Time-resolved approach***. Time dependent effects have to be taken into account in the neutral transport calculation when i) the plasma is evolving significantly on the mean duration of the neutral lifetime (governed by ionization and particle removal) and ii) time scales shorter than the average lifetime duration have to be resolved. In the current EIRENE version, time resolution is implemented by setting a time limit defined by the time step on trajectories, and keeping track of neutral trajectories which exceed the time limit. At the following time step, these trajectories have to be continued in addition to those corresponding to the primary sources. If the time step is small compared to the neutral lifetime, the number of trajectories to track can exceed the capability of the current version of EIRENE. In addition, keeping a given level of statistical noise on the solution can become very demanding compared to a case without time resolution, to the point where it may make the calculation unaffordable in practice – or at least very inefficient. To solve these issues, alternative ways of storing the snapshot densities have to investigated, based on solutions proposed in the literature in different contexts (e.g., multidimensional fits, storing on a velocity grid). The quality of the corresponding approximations has to be assessed. This point is also closely related to the coupling scheme (see ***D1.a***) between the neutral gas module and the plasma code.

b. ***Model for divertor target (W) and FW.*** The NGM based on EIRENE will be coupled to divertor target and first wall models with focus on W as the material relevant for JET, ITER and DEMO. The neutral and plasma interaction with the divertor target and first wall includes processes like sputtering, sticking, adsorption and desorption all of which depend on the state of the target and wall material (temperature, degree of saturation, etc). Thus, a fully self-consistent model requires coupling the NGM-CFD code to a model for the state of the wall and target material containing both the surface layer and the bulk material including possible cooling structures. For this purpose, the NGM-CFD code will be coupled to an existing industry standard code suite providing a finite element model of the wall or target material and structure using the coupling tools developed in task D1.a. The coupling scheme will be fully generic easing its application to different materials modelling code suites. For testing purposes, a simple FEM model for the ITER divertor target W monoblocks will be implemented. Verification runs will be performed for steady and time-dependent situations to ensure the correctness of the coupled NGM-CFD/FEM code. The tools developed and experiences gained within this task will also be relevant for the coupling to the codes developed under TSVV-7.

c. ***Modularisation of EIRENE into NGM.*** As already stated in D1, the NGM will consist of compact numerical HPC-optimized core, free from branching, and a "starter" part preparing a grid and necessary input for the core (further developed mainly in ***D1.a***). Ideally, the core is comprised of a set of volumetric cells with all the data already pre-sorted and condensed down to a minimum. The core requires only a minimal set of input parameters about a cell, excluding general data for the grid and any underlying data except to the ones related to following particles in particular conditions of the selected cell. This will provide the optimal starting point for the HPC optimisation and domain decomposition inside the D1. It will also allow reducing the size of the code related to the main loop and naturally exclude the serial part. To keep the functionality of the EIRENE the procedure of the segregation will be the following. First, we focus on a single selected case (slab for simplicity): the core should run on a data produced by the existing EIRENE through additional output of the currently internal data. Later on one should optimise the core by further unloading of the main loop (e.g. data pre-processing). The core should obtain compact, clear and modern (JSON) input free from branching, but including HPC-related parameters. Further optimisation will continue in ***D1.b,c***. An essential part of the development will be seeking an optimal distribution of the work load between the core and starter, which may need some revisits even later, during the optimisation for HPC or by doing meaningful runs for various fusion devices in ***D5***.

d. ***General code development and maintenance.*** The NGM will have an infrastructure helpful to minimise maintenance effort. The versioning control will be accomplished by a single Git repository, including all code variations, support codes and scripts, documentation, and data (or links in case large volumes are an issue). All options worth of development inside TSVV-5 (a variety of detached versions exist for present-day EIRENE) will be branches from the single main development line. The number of simulation cases should be reduced by selecting the most relevant ones for the project, which are well interlinked and complimentary to each other. For instance, for verification we will use simplified slab cases with parameters directly relevant for the selected validation (actual experiments) and prediction (e.g., ITER). A catalogued storage system for simulations covering those portfolio cases will be provided as well as documentation, master input files etc. Such archival system minimises common effort for establishing the cases, used for different purpose. This procedure also provides additional protection against code changes and bugs, and reduces the total number of simulations to be carried out. Well-defined set of cases will ease interfacing with other TSVVs (***D1.a***).

e. ***Adjoint approach.*** In plasma-edge simulation tools such as the NGM, simulated outputs often depend on a large number of (possibly uncertain) inputs, such as reaction data, surface reflection models, input plasma backgrounds and boundary conditions. Due to the complex physical interactions included in the models, it may be very difficult to assess the sensitivity of simulated outputs to changes in that large amount of input parameters. A direct approach based on finite differences is often practically impossible, due the large number of inputs on the one hand, and the impact of MC noise on the other. A reliable alternative is to use of discrete adjoint sensitivities, which are very robust to MC noise [21]. We will investigate the computation of sensitivities in EIRENE using forward and backward algorithmic differentiation (AD) with the TAPENADE package developed at INRIA; a tool already used successfully to compute sensitivities in B2.5 (SOLPS-ITER) [22]. Making such sensitivities available in the NGM greatly expands the information provided to the modeller, and opens up the way towards rigorous sensitivity analysis, UQ, and automated parameter and design optimization studies. In addition, adjoint simulations allow for efficient computation of output quantities in cases where the MC particles emitted from the 'source' (e.g. recycling surfaces) have small probability to reach the 'detector' (e.g., a remote pumping surface).

D5. Strategy towards a validated predictive capability for integrated fusion reactor modelling for (semi-)detached divertor plasmas. Liaison with TSVV Tasks 3 and 4.

a. ***Validation of CRMs and Lyman photon opacity in JET-ILW, MAGNUM-PSI and PSI-2 plasmas.*** Dedicated measurements of atomic and molecular deuterium emission in the ultra-violet and visible wavelengths range were performed in JET-ILW Ohmic and quasi-stationary MAGNUM-PSI linear plasmas with the purpose of characterising the impact of plasma-ion molecule interaction on the degree of detachment. PSI-2 linear device [23] will complement the MAGNUM-PSI measurements with stable, well-characterized plasma at similarly low plasma temperatures (T_e<1.5 eV), but 3 order of magnitude smaller densities (n_e~1e18 m^{-3} vs. 1e21m^{-3}). Atomic emission of the Lyman (JET only) and Balmer series, and molecular Fulcher band emission were measured in high-recycling and semi-detached conditions to infer the atomic and molecules influxes of tungsten targets, and the ro-vibrational temperatures of deuterium molecules. The photon tracing will allow taking into account opacity effects recently shown to be significant for JET [24] and expected to be even of more importance in ITER/DEMO. The edge code packages EDGE2D-EIRENE (JET only) and SOLPS-ITER are used to simulate these plasmas. Interface to TSVV-3 from D1.a is necessary for that as well as liasing with TSVV-3, 4 on the appropriate fluid and turbulence assumptions. As part of ***D5***, synthetic diagnostics will be implemented into NGM to post-process NGM simulations for the predicted atomic and molecular emissions, permitting direct comparison of the predicted emissions to the corresponding measurements. These activities build upon ***D2.c*** and the development and verification of the isotope model within the NGM development. Furthermore, NGM predictions for distributions of the vibrational quantum states of deuterium molecules and their temperature (rotational state) will be compared to the distributions inferred from the measured spectra. Previous measurements and B2-EIRENE simulations in ASDEX Upgrade with carbon divertor target plates [12] highlighted the role of vibrationally activated hydrogen molecules on the degree of detachment, including the preferential vibrational state due to the release of molecules from the carbon surface. This task/deliverable will re-assess these results in JET-ILW and MAGNUM-PSI, with W as the target plate material, as in ITER and DEMO, which was shown to have a significant impact on the ro-vibrational state of hydrogen molecules [25], [26].

b. **Validating and using the FEM target/FW model.** To verify the coupled NGM-CFD/FEM wall introduced in ***D4.b***, steady state and time-dependent runs will be validated against experimental results from MAGNUM-PSI at DIFFER [27]. This plasma linear device is capable of depositing a similar heat flux to the exposed target than the expected one at ITER. In a first step a validation will be performed for steady state conditions with varying degrees of plasma detachment. In particular, simulated wall temperatures will be validated on experimental data. This will be followed up by validation of time-dependent simulations on the responses observed in

MAGNUM-PSI to transient high heat loads focussing in particular on reattachment and the evolution of the wall properties (temperature, outgassing, sputtering, etc).

c. **DEMO simulations using FKH.** Edge plasma simulations of ITER and DEMO are particularly challenging due to the high densities and resulting collisionalities reached in the divertor. The use of advanced fluid and hybrid methods is expected to drastically speed up the simulations, by avoiding the need to simulate all CX collisions in regions where the neutrals behave as fluid. Through a series of test cases of increasing complexity, we will demonstrate the computational speed-up and accuracy that can be obtained with FKH (see ***D2.a,b***) compared to fully kinetic simulations for DEMO. Test cases will progress from a) slab cases with ITER and DEMO relevant sizes and densities, to b) (scaled) ITER geometries, to c) eventually targeting DEMO geometry and magnetic field.

d. ***Assessment of NGM physics in ITER and DEMO conditions.*** Building on the evaluation of NGM for JET, MAGNUM-PSI and PSI-2 plasmas (***D5.a***), upscaling in major radius to ITER and DEMO size will be used to assess the importance of the added A&M processes and Lyman photon opacity in NGM in reactor-relevant condition. These studies will be conducted by upscaling slab and JET cases in size, power and upstream SOL density. Representative predictive simulations for ITER will demand iterative fluid-NGM runs; also the turbulence effects need to be considered – we will liaison on that with TSVV Tasks 3 and 4. The latter communication will start earlier in the frame of development of the NGM interfaces (***D1.a***) using the portfolio (***D4.d***) cases starting with the simplest, slabs for verification of correctness and efficiency followed by validation in ***D5.a***. The final demonstrative runs for ITER should focus on semi-detached scenario with all newly implemented physics included. Besides testing the physics models, this task permits further assessment of the computational performance of NGM in ITER-size configurations. The latter will demand parallelisation optimisation in ***D1.c*** finished and further support from the ACH HPC.

Table 2. *Measurable results, milestones and risks for SMART deliverables (see the workplan above)*

SMART deliverable	RUs	Measurable result (s)	Subtasks and Milestones to be reached [due date] or [duration]	Known risks incl. related to other activities
[D1.a] **Lean MC code for HPC applications, compatible with TSVV3/4/6 developments**	**CEA, FZJ**	**Speed-up, maintainability and increased optimization potential**	1) Provide "starter" condensing most of EIRENE branching for single geometry option(s), check correctness **[2023].** 2) Assess performance of lean core for relevant geometry options **[24 months].** 3) Interface to TSVV-3 fluid code released **[end of 2025].**	1) Availability and suitability of HPC resources 2) Possible delays in related TSVVs 3) Level of support from ACH
[D1.b] **Domain decomposition for MC solver**	**CEA**	**Reduced memory consumption at node level, CPU load balancing flexibility**	1) demonstrate correctness **[2023]** 2) scaling evaluation using profiling tools and optimizing with support from ACH HPC **[12 months]** 3) run with > 1 billion cells on meaningful cases **[2025]**	1) Availability and suitability to HPC resources 2) Level of support from ACH HPC
[D1.c] **Parallelisation optimization**	**CEA,** **ACH HPC**	**Weak scalability, memory usage**	1) Port NGM on MARCONI, run it on 1 node **[6 months]** 2) Scalable on 100 nodes (any HPC) with flexible regulation of load balancing including tests of different strategies, utilization of domain decompostition and use of profiling tools with support from ACH HPC **[24 months]**. **3)** Demonstrate good scalability for various HPCs, 250+ nodes, various options etc. **[end of 2025]**	1) Progress in code refactoring, 2) Availability of HPC resources and their technical versality 3) Support level from ACH HPC

[D2.a] **Spatial FKH**	**KUL, CEA**	**Completeness of fluid model, speed-up, robustness**	1) Generalization AFN model for drifts and n-n collisions **[15 months]** 2) Generalization AFN model towards multi-species: H/D/T **[12 months]** 3) Optimization of SpH interfacing scheme **[12 months]** 4) Implementation/assessment fluid/hybrid model for molecules **[15 months]**	Some revisit necessity may be revealed by ***D5.c***
[D2.b] **Micro-macro and kinetic-diffusion FKH**	**KUL**	**Speed-up,** **robustness,** **accuracy**	1) Overview and assessment of techniques to reduce bias, cancellation and modelling errors in simplified cases **[15 months]** 2) Implementation of basic KD scheme in EIRENE **[15 months]** 3) Performance assessment of FKH schemes for various density regimes **[2023]** 4) Optimization of FKH schemes in EIRENE **[24 months]** 5) Generalization kinetic-diffusion scheme to multiple species and (scattering) events **[24 months]**	Some revisit necessity may be revealed by ***D5.c***
[D3.a] **Improved AMNS database structure:** IMAS, new ADAS "mdf" formats, unification with other codes incl. ERO); Reduced modesl for PSI, FW isotope content	**FZJ, Aalto U,** **ACH IM**	**Completeness,** **Fraction of particular models validated by NGM applications**	**1)** Incorporate new “mdf” formats recently available in ADAS for molecular data **[12 months]** and test the new CRMs **[2023].** **2)** Unify where possible the database with other codes employed inside TSVVs e.g. ERO2.0, move on using IMAS as a platform **[12 months].** **3)** Provide data and parameters for outgassing, CAPS, wall isotope content etc. based on reduced models, do validation runs **[24 months].**	In 4) selection of reduced models may be a subject of availability
[D3.b] **Improved in content AMNS Database:** reaction and CRM data relevant for detachment, revisited PSI data, index of data used in applications	**FZJ,** **ACH IM** **ACH D**	**Completeness, Data quality** **Fraction of data validated by NGM applications**	1) Compile and incorporate reaction data relevant for ITER/DEMO divertor conditions (low T_e) **[24 moths].** 2) Incorporate spectroscopy and reaction data for H/D/T-containing molecules **[2023].** 3) Revisit erosion and reflection database including CAPS and chemical erosion (SDTrimSP, MD, etc.) **[12 months].** 4) Provide an index of data tested in NGM applications **[2025]** and an overview report **[2027]** on the data quality. 5) Move to IMAS platform (with ACH IM&D) **[3-6 months, timing depend on ACH]**	Level of ACH D support and its usefulness is uncertain. Relevant progress of ADAS filling its molecular data (recent “mdf” format) is uncertain.
[D4.a] **Revisit time dependent scheme (in connection with TSVV 3,4**	**CEA, KUL**	**Noise reduction at given CPU effort**	1) Proof of correctness **[24 months]**. 2) Performance evaluation w.r.t. current implementation **[2023]**.	Depends on code development inside this project including e.g. ***D4.c***
[D4.b] **Coupling of the NGM-CFD code to a Finite Element Model for divertor target / first wall**	**DIFFER**	**Completeness**	1) Provide a simple Finite Element Model for W divertor target (or FW) **[12 months]** 2) Generic coupling scheme in the frame of ***D1.a*** with NGM-CFD with a FEM for W divertor model **[mid 2023]** 3) Perform runs to ensure the correctness of the model and coupling steady state situation **[end of 2021]**	**Depends on *D4.a***

			4) Verification of the coupling in time-dependent runs **[mid of 2023]**	
[D4.c] **Code modulisation: segregation of the compact numeric core and “starter”.**	**FZJ, CEA**	**Completeness** **Release version**	1) Demonstrate compact core working on single application case, with manually prepared input for it **[12 months].** 2) Using experience from 1) provide a run preparation “starter” tool providing a framework to recover full functionality of the initial EIRENE code **[12 months].**	Some revisions may be necessary after work on optimisation for HPC (***D1.a-c***) and even application/verification runs.
[D4.d] **General development of NGM, restructuring (e.g. core segregation) and maintenance of the code**	**FZJ leading,** **all RUs**	**Frameworks introduced** **Frameworks (and content) documented**	**1)** Provide central repository and merge all versions at least as branches **[2024].** **2)** Provide code documentation **[2027]** and universal GUI-based visualization tools **[mid 2023 + later updates].** 3) Portfolio of simulation cases and runs databank **[mid 2023 + later updates]**. 4) Provide CI cases (related to portfolio of simulation cases – see below) **[2023 + later updates]**. 5) Code refactoring and general restructuring incl. segregation of the compact core **[2001 – conceptual design, 2003 – after some iterations with D1.a]**.	Maintenance effort difficult to estimate: sufficient manpower may be an issue
[D4.e] **Adjoint approach**	**KUL**	**Accuracy**	1) Interfacing of Eirene with Tapenade in forward AD mode **[12 months]** 2) Interfacing of Eirene with Tapenade in backward AD mode **[12 months]** 3) Assessment of bottlenecks for efficient use of AD and in EIRENE and coupled EIRENE-CFD packages; identification of options to improve efficiency **[12 months]** 4) Implementation and testing of most promising AD options identified in 3) **[24 months]**	Obsolete FORTRAN features not supported by Tapenade may require iterations with ***D4.d***
[D5.a] **Validation of refined CRMs in JET-ILW, MAGNUM-PSI and PSI-2 plasmas; investigate isotope effect (H/D/T plasma) on detachment.**	**Aalto Univ., DIFFER, FZJ**	**NGM validity assessment against experimental result, performance assessment for actual experimental devices**	1) Compare NGM predicted against experimentally inferred influxes, ro-vibrational temperatures, and Lyman opacity from JET-ILW Ohmic, MAGNUM-PSI and PSI-2 **[24 months]** 2) Elucidate dependencies of influxes and Lyman opacity on plasma conditions **[12 months]** 3) Evaluate particle, momentum and power losses due to plasma-atom and plasma-molecule interaction **[12 months]** 4) Assess higher-power/higher density, H-mode like density regime **[12 months]**	Depends on ***D2.c***
[D5.b] **Validation of NGM-CFD/FEM coupled code with MAGNUM-PSI experimental data**	**DIFFER**	**Validation of** **Steady state and time-dependent: wall temperature**	1) Setup of validation case **[12 months]** 2) validation of the coupled model in steady state runs with experimental data from MAGNUM-PSI **[2022]** 3) validation of the coupled model in time-dependent runs with experimental data from MAGNUM-PSI **[end 2023]** 4) extrapolation of modelling to divertor tokamaks **[24 months]**	Depends on ***D1.a*** and availability and quality of the fluid simulations for linear device MAGNUM-PSI
[D5.c] **Demonstrate advantages of FKH**	**KUL**	**Speed-up / accuracy**	1) Application/assessment of FKH for slab DEMO **[12 months]** 2) Application/assessment of FKH for real DEMO (scaled ITER) geometry **[12 months]**	Availability and numerical stability of models reached in ***D2.c***; underlying

on predictive case for DEMO			3) Performance assessment FKH for ITER/DEMO relevant conditions **[end of 2025]**	data refinement in ***D3.a*** and ***D3.b***
[D5.d] **Assessment of NGM physics and performance by ITER predictions**	**Aalto Univ., FZJ** **ACH HPC**	**Demonstration of NGM in reactor-relevant conditions, assessment of relevance of physics models**	1) Perform predictive upscaled slab and JET NGM (SOLPS-ITER in collaboration with TSVV 3) simulations **[12 months]**, assess the inclusion of refined physics models **[12 months].** **2)** Assess HPC performance of NGM for full-ITER scale simulations **[6 months].** **3)** Perform meaningful runs for seeded semi-detached ITER scenario with variation of degree of detachment and recycling conditions. Do reusability checks and compare with experience in existing devices including JET-ILW **[early 2027].**	Successful model development under ***D2.c*** and validation under ***D5.a***. HPC optimisation and adjoint runs are needed – ***D1.c***, ***D4.e.*** SOLPS-ITER interface should be ready within ***D1.a***

Project timeline

Important notes: the timeline assumes a starting date 1.1.2021. It is also submitted to IMS as a separate PDF-file with a better resolution.

Formal reporting will be done for each call deliverable D1-D5 by 3 marked dates (green arrows at the top of ***fig. 2***) based on results obtained earlier in the project (vertical bars). In addition, we will summarize the TSVV work outcome in three topical overview papers (or preprints): 1) code description incl. use of HPC; 2) underlying data description; and 3) physics in the code relevant for ITER/DEMO extrapolated from existing devices. The corresponding authors are indicated by their initials (“MG”, “YM”, “DB” etc.).

The strategy presented in the timeline given in ***fig. 2*** is for maximal possible duration of the TSVV-5: 5+2 years. The 1st and 2nd interim reports indicated will allow assessing the progress of the work and making decision on a potential project extension up to 7 years.

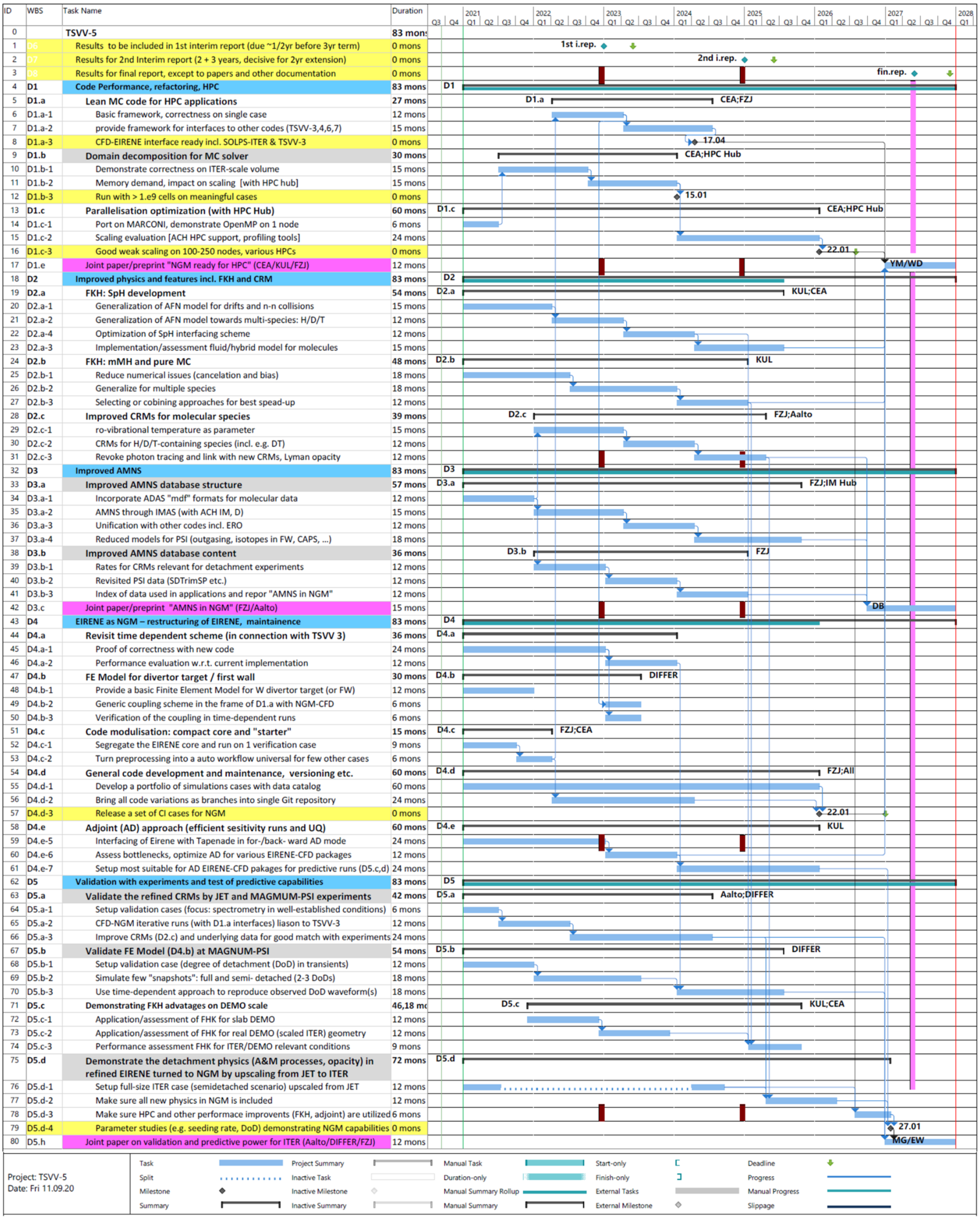
The primary goals for the five-year duration of the project are the following:

1) The existing neutral Monte-Carlo code EIRENE will be modernised, improved by its structure, and converted to a Neutral Gas Module to be used by other TSVVs. HPC adaptation will be assessed and implemented.
2) The collisional radiative model, the target finite elemental model and fundamental atomic and molecular data will be updated, and the models validated.
3) Fluid-kinetic hybridisations methods will be developed and assessed for DEMO-scale cases.

The following potential tasks for extension of the project beyond the 5th year have been identified:

1) D1.a: expansion of interface to CFD-NGM for 1-3 for adaption of NGM in fluid codes
2) D3: extension of AMNS data and reduced models for PSI.
3) D5a: extension of validation in linear devices MAGNUM-PSI and PSI-2
4) D5d, D5b: Optimized HPC demonstration on ITER scale
5) D2: Further enhancement of capabilities of FKH, depending on progress and needs identified in first period (e.g. radiation transport)
6) D4: Extension adjoint approach to coupled EIRENE-CFD applications

These tasks allow finalisation of the NGM development, including interface framework development parallelisation optimisation, iteration of model development with verification and validation, and sensitivity studies of the new models for JET and ITER plasmas.



ID	WBS	Task Name	Duration
0		**TSVV-5**	**83 mons**
1	D6	Results to be included in 1st interim report (due ~1/2yr before 3yr term)	0 mons
2	D7	Results for 2nd Interim report (2 + 3 years, decisive for 2yr extension)	0 mons
3	D8	Results for final report, except to papers and other documentation	0 mons
4	**D1**	**Code Performance, refactoring, HPC**	**83 mons**
5	**D1.a**	**Lean MC code for HPC applications**	**27 mons**
6	D1.a-1	Basic framework, correctness on single case	12 mons
7	D1.a-2	provide framework for interfaces to other codes (TSVV-3,4,6,7)	15 mons
8	D1.a-3	CFD-EIRENE interface ready incl. SOLPS-ITER & TSVV-3	0 mons
9	**D1.b**	**Domain decomposition for MC solver**	**30 mons**
10	D1.b-1	Demonstrate correctness on ITER-scale volume	15 mons
11	D1.b-2	Memory demand, impact on scaling [with HPC hub]	15 mons
12	D1.b-3	Run with > 1.e9 cells on meaningful cases	0 mons
13	**D1.c**	**Parallelisation optimization (with HPC Hub)**	**60 mons**
14	D1.c-1	Port on MARCONI, demonstrate OpenMP on 1 node	6 mons
15	D1.c-2	Scaling evaluation [ACH HPC support, profiling tools]	24 mons
16	D1.c-3	Good weak scaling on 100-250 nodes, various HPCs	0 mons
17	D1.e	Joint paper/preprint "NGM ready for HPC" (CEA/KUL/FZJ)	12 mons
18	**D2**	**Improved physics and features incl. FKH and CRM**	**83 mons**
19	**D2.a**	**FKH: SpH development**	**54 mons**
20	D2.a-1	Generalization of AFN model for drifts and n-n collisions	15 mons
21	D2.a-2	Generalization of AFN model towards multi-species: H/D/T	12 mons
22	D2.a-4	Optimization of SpH interfacing scheme	12 mons
23	D2.a-3	Implementation/assessment fluid/hybrid model for molecules	15 mons
24	**D2.b**	**FKH: mMH and pure MC**	**48 mons**
25	D2.b-1	Reduce numerical issues (cancelation and bias)	18 mons
26	D2.b-2	Generalize for multiple species	18 mons
27	D2.b-3	Selecting or cobining approaches for best spead-up	12 mons
28	**D2.c**	**Improved CRMs for molecular species**	**39 mons**
29	D2.c-1	ro-vibrational temperature as parameter	15 mons
30	D2.c-2	CRMs for H/D/T-containing species (incl. e.g. DT)	12 mons
31	D2.c-3	Revoke photon tracing and link with new CRMs, Lyman opacity	12 mons
32	**D3**	**Improved AMNS**	**83 mons**
33	**D3.a**	**Improved AMNS database structure**	**57 mons**
34	D3.a-1	Incorporate ADAS "mdf" formats for molecular data	12 mons
35	D3.a-2	AMNS through IMAS (with ACH IM, D)	15 mons
36	D3.a-3	Unification with other codes incl. ERO	12 mons
37	D3.a-4	Reduced models for PSI (outgasing, isotopes in FW, CAPS, …)	18 mons
38	**D3.b**	**Improved AMNS database content**	**36 mons**
39	D3.b-1	Rates for CRMs relevant for detachment experiments	12 mons
40	D3.b-2	Revisited PSI data (SDTrimSP etc.)	12 mons
41	D3.b-3	Index of data used in applications and repor "AMNS in NGM"	12 mons
42	D3.c	Joint paper/preprint "AMNS in NGM" (FZJ/Aalto)	15 mons
43	**D4**	**EIRENE as NGM – restructuring of EIRENE, maintainence**	**83 mons**
44	**D4.a**	**Revisit time dependent scheme (in connection with TSVV 3)**	**36 mons**
45	D4.a-1	Proof of correctness with new code	24 mons
46	D4.a-2	Performance evaluation w.r.t. current implementation	12 mons
47	**D4.b**	**FE Model for divertor target / first wall**	**30 mons**
48	D4.b-1	Provide a basic Finite Element Model for W divertor target (or FW)	12 mons
49	D4.b-2	Generic coupling scheme in the frame of D1.a with NGM-CFD	6 mons
50	D4.b-3	Verification of the coupling in time-dependent runs	6 mons
51	**D4.c**	**Code modulisation: compact core and "starter"**	**15 mons**
52	D4.c-1	Segregate the EIRENE core and run on 1 verification case	9 mons
53	D4.c-2	Turn preprocessing into a auto workflow universal for few other cases	6 mons
54	**D4.d**	**General code development and maintenance, versioning etc.**	**60 mons**
55	D4.d-1	Develop a portfolio of simulations cases with data catalog	60 mons
56	D4.d-2	Bring all code variations as branches into single Git repository	24 mons
57	D4.d-3	Release a set of CI cases for NGM	0 mons
58	**D4.e**	**Adjoint (AD) approach (efficient sesitivity runs and UQ)**	**60 mons**
59	D4.e-5	Interfacing of Eirene with Tapenade in for-/back- ward AD mode	24 mons
60	D4.e-6	Assess bottlenecks, optimize AD for various EIRENE-CFD packages	12 mons
61	D4.e-7	Setup most suitable for AD EIRENE-CFD pakages for predictive runs (D5.c,d)	24 mons
62	**D5**	**Validation with experiments and test of predictive capabilities**	**83 mons**
63	**D5.a**	**Validate the refined CRMs by JET and MAGMUM-PSI experiments**	**42 mons**
64	D5.a-1	Setup validation cases (focus: spectrometry in well-established conditions)	6 mons
65	D5.a-2	CFD-NGM iterative runs (with D1.a interfaces) liason to TSVV-3	12 mons
66	D5.a-3	Improve CRMs (D2.c) and underlying data for good match with experiments	24 mons
67	**D5.b**	**Validate FE Model (D4.b) at MAGNUM-PSI**	**54 mons**
68	D5.b-1	Setup validation case (degree of detachment (DoD) in transients)	12 mons
69	D5.b-2	Simulate few "snapshots": full and semi- detached (2-3 DoDs)	18 mons
70	D5.b-3	Use time-dependent approach to reproduce observed DoD waveform(s)	18 mons
71	**D5.c**	**Demonstrating FKH advatages on DEMO scale**	**46,18 mo**
72	D5.c-1	Application/assessment of FHK for slab DEMO	12 mons
73	D5.c-2	Application/assessment of FHK for real DEMO (scaled ITER) geometry	12 mons
74	D5.c-3	Performance assessment FHK for ITER/DEMO relevant conditions	9 mons
75	**D5.d**	**Demonstrate the detachment physics (A&M processes, opacity) in refined EIRENE turned to NGM by upscaling from JET to ITER**	**72 mons**
76	D5.d-1	Setup full-size ITER case (semidetached scenario) upscaled from JET	12 mons
77	D5.d-2	Make sure all new physics in NGM is included	12 mons
78	D5.d-3	Make sure HPC and other performace improvents (FKH, adjoint) are utilized	6 mons
79	D5.d-4	Parameter studies (e.g. seeding rate, DoD) demonstrating NGM capabilities	0 mons
80	D5.h	Joint paper on validation and predictive power for ITER (Aalto/DIFFER/FZJ)	12 mons

Project: TSVV-5
Date: Fri 11.09.20

Figure 2. *Proposed timeline for TSVV-5: "D1-D5" correspond to call deliverables and "DX.a,b,c,…" to the smart deliverables from the table 2, however the titles are reduced for readability, subprojects and milestones are somewhat simplified in some cases.*

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*

  Substantial CPU time and access to a large number of nodes will be necessary for the optimisation and testing of the domain decomposition schemes. Weak scaling test on 0.1h selected case (minimum to keep the impact of serial part negligible) with (512 + 256 + 128 + 64 + 32 + 16) nodes * 48 cores/node will demand **4.876 core-h**
  Assuming that the test should be run ~20 times until optimization is obtained, this gives ~0.1 Mln core-h. However, as stated in ***D1.a***, we need also develop the general framework and particular interfaces to the codes employed in TSVV-3 and others. Just the fluid codes (B2, EMC3, Edge2D, SOLEDGE3X, …) may demand repeating of the exercise for 10 times giving that some revisits may be necessary after more experience is gained. Therefore, starting from 2022 (after code restructuring in ***D4.c*** is finished) TSVV-5 may need ~0.5 Mln core-h for optimization tests alone.

  Based on experience with coupled edge-fluid/EIRENE cases, JET and ITER simulations can take up to several months to converge, including parallelised versions of EIRENE. The slow conversion is partly due to the fluid part of the code (single node, lack of domain decomposition (TSVV-3)), and the high number of grid cells, the large number of EIRENE particles and the number of iterations between the fluid code and EIRENE required to achieve convergence. Hence, significant reductions of the computational time inside NGM as proposed above will ultimately reduce the overall speed of coupled edge-fluid/EIRENE simulations, and thereby permit a larger number of production runs.

  The productive runs for DEMO and ITER will also likely be very resource demanding. However, the precise estimation can be done only after the parallelization scheme will be fully optimized in the frame of ***D1.c*** and will heavily depend on the size of grids used (2D vs 3D, and resolution), thus increase gradually with progress of plasma codes during the project.

- *Anticipated number of nodes required (which partition?)*
  We will need maximal allowed number of nodes to test the weak scaling: up to 512 nodes on 'skl_fua_prod' partition. DEMO and ITER performance tests will also demand maximal performance available for a standard user.

- *Special requirements (optional)*
  We aim to develop the NGM useful for massive simulations including in various coupling schemes, thus we aim to avoid any special requirements except to the sheer CPU power determined by the reactor volumes, densities, complexity of geometry and other factors.
  *Available memory should not be a direct limitation due to domain decomposition in (**D1.b**), however can affect the resulting performance and flexibility for optimisation.*

Expected long-term requirements of HPC resources?

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

Expected level of support is given in table .1

The Advanced Computing Hubs (ongoing call, Ref. PMU/1740) will cover the following topics and activities:

- *Production runs for NGM verification against present EIRENE and for JET validation cases*

  Assistance with standalone NGM as well as liasing with TSVV 3 for coupled edge fluid/NGM production runs for JET, MAGNUM, ITER, DEMO (optimize for performance) will be required within D5.b-d.

- *High Performance Computing (scalable algorithms, code parallelization and performance optimization, code refactoring, GPU-enabling etc.)*

  From an ACH for HPC support is requested on the following items:
  (i) Most important and effort demanding will be assistance during the work on the optimized parallelization in **D1.c** and related to that (also useful for overcoming the memory limitations) domain decomposition **D1.b**. In particular, the code profiling with the best suitable tools and incorporation of most up-to-date parallelization techniques, command systems, data formats and libraries. Guidance from the HPC experts on the available HPC architectures (e.g. MARCONI), with an outlook to expected future developments and constraints, will also be of value.
  (ii) Some assistance and consulting will be helpful already during the code restructuring including **D1.a** and **D4.c,** which are preceding steps for the work done in (i).

- *Integrated Modelling and Control (code adaptation to IMAS, IMAS framework development, code integration etc.)*

  From an Integrated Modelling and Control ACH support is requested on the following items:
  (i) for code adaptation to the IMAS (Integrated Modelling and Analysis Suite) platform. This includes data storage in IMAS data base and standardization of data exchange between NGM and other codes in terms of IDSs (Interface Data Structures).
  (ii) for the coupling framework of the NGM to other codes [**D1.a**].
  (iii) for porting of the newly developed AMNS data to the relevant IMAS data base [**D3.a and b**]
  (iv) for support in the implementation of newly developed algorithms for the different Fluid Kinetic Hybrid schemes **[D2.a and b**]

- *Data Management (open access, data management, data analysis tools, aspects of AI and VVUQ etc.)*

  From an ACH D support is requested on the following items:
  (i) in handling of massive additional AMNS data to be added in a controllable way to the EIRENE-based NGM [**D3a,b**] including logging and indexing its use throughout the simulation cases.
  (ii) in development of the cataloged repository for the simulated data, which may have huge volumes and high versality **[D4.d**]

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