EUROfusion

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

Title (c.f. Annex-2)	***Plasma-Wall Interaction in DEMO***
TSVV Task leader (name/e-mail)	***Dmitry Matveev / d.matveev@fz-juelich.de***
Lead beneficiary	***FZJ (Germany)***
Project duration	***5 years***

TSVV Task leader

Name:	Dmitry Matveev
Institution:	Forschungszentrum Juelich
Street Address:	Wilhelm-Johnen-Strasse
City:	Juelich
Country:	Germany
Email:	d.matveev@fz-juelich.de
Phone:	+49 2461-61-96625

TSVV Task team members [other than the leader]

Name:	Juri Romazanov
Institution:	Forschungszentrum Juelich
Street Address:	Wilhelm-Johnen-Strasse
City:	Juelich
Country:	Germany
Email:	j.romazanov@fz-juelich.de
Phone:	+49 2461-61-2631

Name:	Sebastian Rode (PhD student)
Institution:	Forschungszentrum Juelich
Street Address:	Wilhelm-Johnen-Strasse
City:	Juelich
Country:	Germany
Email:	se.rode@fz-juelich.de
Phone:	+49 2461-61-2631

Name:	Klaus Schmid
Institution:	Max-Planck-Institut für Plasmaphysik
Street Address:	Boltzmannstrasse 2
City:	Garching
Country:	Germany
Email:	klaus.schmid@ipp.mpg.de
Phone:	+49 89 3299 2228

Name:	Udo v. Toussaint
Institution:	Max-Planck-Institut für Plasmaphysik
Street Address:	Boltzmannstrasse 2
City:	Garching
Country:	Germany
Email:	udo.v.toussaint@ipp.mpg.de
Phone:	+49 89 3299 1817

Name:	Fredric Granberg
Institution:	University of Helsinki
Street Address:	Gustaf Hällströmin katu 2, P.O. Box 43
City:	Helsinki
Country:	Finland
Email:	fredric.granberg@helsinki.fi
Phone:	+358 503112603

Name:	Alvaro Lopez-Cazalilla
Institution:	University of Helsinki
Street Address:	Gustaf Hällströmin katu 2, P.O. Box 43
City:	Helsinki
Country:	Finland
Email:	alvaro.lopezcazalilla@helsinki.fi
Phone:	+358 503112603

Name:	Aleš Podolník
Institution:	Institute of Plasma Physics of the CAS
Street Address:	Za Slovankou 1782/3
City:	Prague
Country:	Czech Republic
Email:	podolnik@ipp.cas.cz
Phone:	+420 266 05 3569

Name:	David Tskhakaya
Institution:	Institute of Plasma Physics of the CAS
Street Address:	Za Slovankou 1782/3
City:	Prague
Country:	Czech Republic
Email:	tskhakaya@ipp.cas.cz
Phone:	+420 266 05 3562

Name:	Michael Komm
Institution:	Institute of Plasma Physics of the CAS
Street Address:	Za Slovankou 1782/3
City:	Prague
Country:	Czech Republic
Email:	komm@ipp.cas.cz
Phone:	+420 266 05 3395

Name:	Svetlana Ratynskaia
Institution:	KTH Royal Institute of Technology
Street Address:	*Teknikringen 29, SE-100 44*
City:	Stockholm
Country:	Sweden
Email:	srat@kth.se
Phone:	+46 8 790 91 21

Name:	Panagiotis Tolias
Institution:	KTH Royal Institute of Technology
Street Address:	Teknikringen 29, SE-100 44
City:	Stockholm
Country:	Sweden
Email:	tolias@kth.se
Phone:	+46 8 790 76 89

Name:	Ladislas Vignitchouk
Institution:	KTH Royal Institute of Technology
Street Address:	Teknikringen 29, SE-100 44
City:	Stockholm
Country:	Sweden
Email:	ltrvi@kth.se
Phone:	+46 8 790 76 90

Name:	Emil Thoren
Institution:	KTH Royal Institute of Technology
Street Address:	Teknikringen 29, SE-100 44
City:	Stockholm
Country:	Sweden
Email:	emitho@kth.se
Phone:	+46 8 790 76 90

Name:	Jernej Kovačič
Institution:	Jožef Stefan Institute
Street Address:	Jamova cesta 39
City:	Ljubljana
Country:	Slovenia
Email:	jernej.kovacic@ijs.si
Phone:	+386 1 5885 413

Name:	Jonathan Mougenot
Institution:	Sorbonne Paris Nord University - LSPM
Street Address:	99 av. J.B. Clément, 93430
City:	Villetaneuse
Country:	France
Email:	jonathan.mougenot@lspm.cnrs.fr
Phone:	+33 1 49 40 34 80

Name:	Yann Charles
Institution:	Sorbonne Paris Nord University - LSPM
Street Address:	99 av. J.B. Clément, 93430
City:	Villetaneuse
Country:	France
Email:	yann.charles@univ-paris13.fr
Phone:	+33 1 49 40 34 61

Name:	Christian Grisolia
Institution:	CEA - IRFM
Street Address:	CEA Cadarache, 13108
City:	Saint-Paul-lez-Durance
Country:	France
Email:	christian.grisolia@cea.fr
Phone:	+33 4 42 25 43 78

Name:	Etienne Hodille
Institution:	CEA - IRFM
Street Address:	CEA Cadarache, 13108
City:	Saint-Paul-lez-Durance
Country:	France
Email:	etienne.hodille@cea.fr
Phone:	+33 4 42 25 43 78

Name:	Rémi Delaporte-Mathurin
Institution:	CEA – IRFM & USPN
Street Address:	99 av. J.B. Clément, 93430
City:	Villetaneuse
Country:	France
Email:	remi.delaporte-mathurin@lspm.cnrs.fr
Phone:	+33 1 49 40 36 25

Relevant skills and experiences of the TSVV Task team

The members of the TSVV team have extensive and long-lasting experience in computational plasma physics and modelling of different aspects of plasma-wall interactions in contemporary fusion devices and for ITER, which are briefly summarized in the following tables for each participating research unit and each team member.

Research unit	***Skills and experiences***
FZJ	Modelling of impurity transport and PWI in JET, W7X, ITER with highly parallel full 3D MC code ERO2.0 (code development and application). Fuel retention modelling with CRDS code.
IPP	Development and application of binary collisions codes of SDTrimSP code family for assessment of PWI data regarding reflection, sputtering and morphology effects (surface roughness). Fuel retention modelling with TESSIM-X code. UQ and AI expertise in application to PWI data.
VR / KTH	Modelling of wall response to transient heat loads. Melting, melt motion and re-solidification with parallel code MEMOS-U. Analysis of dust mobilization and melt splashing probability. Transport of melt droplets and mobilized dust with MIGRAINe code.
IPP.CR	Kinetic (PIC+MC) modelling of complex plasma sheath (divertor plasma) with highly parallel codes of SPICE and BIT code families (code development and application).
JSI	Kinetic (PIC) modelling of static and dynamic SOL with BIT code (application and development).
CEA / USPN	Fuel retention modelling with MHIMS code and 3D finite element codes FESTIM and ABAQUS.
VTT / Helsinki	More than 2 decades experience in development of interatomic potentials, MD and KMC modelling for assessment of PWI data regarding reflection, sputtering and damage creation.

Team member (RU)	***Relevant expertise***
Dmitry Matveev (FZJ)	ITER Science Fellow on the task of fuel retention management, has background in ERO modelling, and develops and maintains the CRDS code.
Jury 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.
Sebastian Rode (FZJ)	Finalizes his master project on the implementation of the guiding center approximation into the ERO2.0 code and has therefore a direct hands-on experience with the program. He will continue as a PhD student at FZJ.
Klaus Schmid (IPP)	ITER Science Fellow on the task of fuel retention management, EUROFusion sub-project leader for WP PFC SP3 "PWI Processes II: fuel retention, fuel removal and material damage" that is, in particular, focused on the formation of defects in W by neutron irradiation, both experimentally and through modeling. The experiments performed as

	part of SP3 have led to a model understanding as to which level defects are generated as function of damage (DPA) and temperature and how these defects are stabilized by the presence of hydrogen species during irradiation. Develops and maintains the TESSIM-X code.
Udo v. Toussaint (IPP)	The principal investigator in the Pilot-project on "Reduced Complexity Models for UQ" of the Helmholtz society. His group has developed several codes on non-intrusive uncertainty quantification. In the past decade IPP has started several initiatives on UQ in fusion research in experiments and modelling. In particular, the 1D SDTrimSP code has already been used as a model code to study UQ methods for sputtering processes. Maintains and develops the SDTrimSP-3D code.
Fredric Granberg (VTT)	Post-Doc at the University of Helsinki, focusing on high dose damage in both conventional and novel structural fusion relevant materials, and sputtering investigations of fusion relevant wall and diagnostics materials, by computational means. The group at Univ. Helsinki maintains the PARCAS code and explained swift chemical sputtering mechanisms and has developed analytical and machine-learning interatomic potentials allowing for simulations of plasma-material interactions for ITER and DEMO first wall materials.
Alvaro Lopez-Cazalilla (VTT)	Post-Doc at the University of Helsinki, focusing mainly on studying sputtering of rough surfaces by computational means. He did his master project on the effects of He in plasma facing materials. He obtained his PhD in 2019 studying nano-patterning formation under ion irradiation using molecular dynamics (PARCAS) and Binary Collisions Approximation methods.
§ Michael Komm (IPP.CR)	Researcher at IPP Prague and a co-developer of SPICE 2D and 3D codes. In the past, he used these codes to investigate plasma interaction with castellated PFCs, behavior of various types of probes and effects of thermionic emission from hot tungsten PFCs. He is currently investigating the models of secondary electron emission and electron backscattering in SPICE2 and the influence of Coulomb collisions on Debye sheath and magnetic pre-sheath.
Aleš Podolník (IPP.CR)	Post-Doc at IPP Prague, his topics include particle-in-cell simulations of edge plasma using the code SPICE in 2D and 3D geometries aimed mostly at sheath studies with respect to studies of sheath expansion effect on electric probe measurements. Maintains and co-develops the SPICE code.
§ David Tskhakaya (IPP.CR)	Researcher at IPP Prague, the author of BIT1, BIT2 and BIT3 codes, has more than 20 year experience in kinetic study of the fusion relevant plasma edge.
Jernej Kovačič (JSI)	Researcher at the JSI, has been involved in several EUROfusion tasks in recent years. His main research topics are kinetic properties of the tokamak SOL, which he approaches with numerical and experimental tools. Recently he has been working on the parallel filamentary transport simulations and on the effects of the divertor thermionic emission on the SOL plasma, employing the massively parallel fully kinetic BIT1 code.
Svetlana Ratynskaia (VR)	Professor at KTH, Stockholm, whose expertise of relevance to this project concerns dust-plasma interaction, contact and impact mechanics, free-surface liquid metal flows with phase transitions.

Panagiotis Tolias (VR)	Researcher at KTH, Stockholm, whose expertise of relevance to this project concerns surface physics, electron emission physics, liquid metal properties, and contact and impact mechanics.
Ladislas Vignitchouk (VR)	Researcher at KTH, Stockholm, whose expertise of relevance to this project concerns numerical modelling of free-surface MHD flows with phase transitions and of dust-plasma and dust-wall interaction.
Emil Thorén (VR)	Post-Doc at KTH, Stockholm, whose expertise of relevance to this project concerns numerical modelling of free-surface liquid metal flows with phase transitions.
Jonathan Mougenot (CEA)	ITER Science Fellow on the task of fuel retention management, contributes to development of fuel retention codes (HIIPC, ABAQUS and FESTIM) to highlight multidimensional and mechanical field effects on diffusion and retention in PFC.
Yann Charles (CEA)	Expert on Finite Element Modelling developments especially in the context of hydrogen diffusion and trapping, coupled with thermo-mechanical fields (including plasticity), in metallic structures. He develops and maintains a retention code based on ABAQUS finite element commercial software.
Christian Grisolia (CEA)	Expert on diffusion and permeation modelling in PFC. He contributes to the development of MHIMS and FESTIM codes.
Etienne Hodille (CEA)	Post-Doc at the CEA focusing on the diffusion/retention modelling. During his PhD (2013-2016) he developed the MHIMS code and continues to maintain it.
Rémi Delaporte-Mathurin (CEA)	PhD candidate of the Sorbonne Paris Nord University focusing on the multiscale modelling of diffusion H and He in PFC, develops and maintains the FESTIM code.

§ Consultants who expressed their interest to participate in discussions but cannot be directly included in the task team due to minimal commitment requirement (see also the next section with commitments of the TSVV Task team members).

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

Task participation by research units p.a. average over 5 years

Research unit	*Commitment*	*Expertise*
ACH	2.0 ppy	HPC, IMAS, AI (can be partly fulfilled by the team)
IPP.CR	0.5 ppy	PIC
JSI	0.5 ppy	PIC
VTT	0.5 ppy	PWI
FZJ	2.0 ppy	Task leader, ERO2.0, retention
CEA	1.8 ppy	Retention
IPP	1.2 ppy	PWI, retention
VR	1.5 ppy	Dust, transients
Total	**10 ppy**	

The above-mentioned commitments will be distributed among team members as listed in the following table:

Team member	***Research unit***	***Commitment (PM)***				
		2021	***2022***	***2023***	***2024***	***2025***
ACH	ACH	32	19	20	26	20
Dmitry Matveev	FZJ	9	6	6	6	6
*Juri Romazanov			**4**	6	6	6
Sebastian Rode		9	9	6	6	6
NN (PhD or Post-Doc)		6	6	6	6	6
Aleš Podolník	§ IPP.CR	6	6	6	6	6
Jernej Kovačič	JSI	6	6	6	6	6
Fredric Granberg	VTT		6	6	6	6
Alvaro Lopez-Cazalilla		6				
**Jonathan Mougenot	CEA	**5**	**5**	**5**	**5**	**5**
**Yann Charles		**5**	**5**	**5**	**5**	**5**
Christian Grisolia		6	6	6	6	6
Etienne Hodille		6	6	6	6	6
***Rémi Delaporte-Mathurin		6	6			
Klaus Schmid	IPP	6	6	6		6
Udo von Toussaint			12	12	12	12
Svetlana Ratynskaia	VR	6	6	6	6	6
Panagiotis Tolias		6	6		6	6
Ladislas Vignitchouk		6	6	6	6	6
Emil Thorén				6		
Total (w/o ACH)		**88**	**101**	**100**	**94**	**100**
Total (w/ ACH)		**120**	**120**	**120**	**120**	**120**

* Juri Romazanov holds EUROfusion ER grant until 31.03.2022, therefore his commitment in 2022 is limited to the remaining months shared between TSVV#6 and TSVV#7. For his indispensable expertise with the ERO2.0 code and 6 PM commitment in the following years, we hope that this exception is justified. Also during the first year of the project his participation in discussions as a consultant will be very helpful, in particular to adapt the achievements within the ER grant to DEMO applications.

** Jonathan Mougenot and Yann Charles represent the Université Sorbonne Paris Nord (USPN) and have imposed teaching obligations of 6 PM. For administrative reasons they are not allowed to commit more than 5 PM to external projects. Since this is a common situation for all French Universities, we hope that this minimal deviation from the minimal commitment requirement is well justified.

*** Rémi Delaporte-Mathurin is covered by other means therefore his 6 PM commitment in 2021 and 2022 is not included in the calculation of the total.

§ David Tskhakaya and Michael Komm, both affiliated with IPP.CR, are experts in PIC modelling and have indicated their interest in participating to the discussions during the course of the project as advisors. For their strong expertise in the subject, in particular as authors and/or main contributors to BIT and SPICE codes development, their consultancy will be very much appreciated. It is the minimal commitment requirement for TSVVs that does not allow to include them as direct participants in the task. Their short profiles are nevertheless included in the team members table in the previous section (see “Relevant skills and experiences of the TSVV Task team“).

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

1. Introduction

Plasma-wall interactions (PWI) in DEMO will have a strong impact on the lifetime of plasma-facing components (PFC), reactor safety, and availability of the plant. As critical issues material erosion and damage, impurity generation, formation and destabilisation of deposited layers, and tritium retention can be identified. As a vital input for the DEMO design team for the conceptual design review (2023), assessment of safety-relevant information regarding first-wall and divertor erosion, dust production and fuel inventory, including the role of transient events, by means of an integrated modelling approach represents the aim of the proposed project.

We identify the following joint objectives relevant for PWI in DEMO and for the DEMO conceptual design review:
O1. Assessment of steady-state W erosion rates for the first wall, limiters and divertor.
O2. Mapping of preferential W re/co-deposition locations.
O3. Assessment of PFC response to transients in terms of melting and splashing.
O4. Assessment of dust mobilization from likely dust/droplet production sites.
O5. Assessment of W erosion rates for locations affected by transients.
O6. Assessment of tritium in-vessel inventory (co-deposition and bulk retention).

Currently there is no single code that can address different aspects of PWI at all relevant scales and operation scenarios, including normal and off-normal transients. However, there is an existing set of powerful and validated tools that not only can address particular PWI aspects in DEMO, but also can interact with each other by means of data exchange in order to provide boundary conditions for respective sub-systems and increase the confidence of the overall result.

According to the above list of objectives and competences of team members, we propose to address each of the objectives with existing codes in a phased approach, in which the first phase is foreseen to deliver preliminary results with existing codes and available input data, the second phase aims at further elaboration of the input data and code capabilities for improved deliverables, and the third phase is seen as integration and optimization of the code package as a final product for DEMO PWI modelling. Each phase implies data and code development and validation work in preparation for the subsequent phase. Phasing of the overall project has to be seen in terms of availability of particular deliverables and extension of the complexity of PWI phenomena addressed rather than as a staged timeline.

2. Approach to steady state PWI

Plasma-wall interactions are strongly coupled to the transport of plasma and neutrals in the scrape-off layer (SOL) and governed by the particle and heat fluxes to the surface, therefore a consistent plasma background is essential for PWI and impurity transport modelling. Such plasma backgrounds are typically provided by specialized simulation tools such as SOLPS-ITER [Wie15], in particular employed by ITER Organization (IO) to study ITER plasma boundary physics and tokamak performance [Kav20]. Due to complexity of the task of plasma edge modelling and the versatility of processes that should be addressed within the current proposal, it is not feasible to include plasma background modelling in the current project. Moreover, SOLPS-ITER modelling for DEMO plasma represents an already ongoing project within WP PMI. Thus it is anticipated that the background plasma, the wall geometry and material choices represent an external input from related work packages, in particular WP DES.

Post-processing of SOLPS results is essential to provide respective interfaces to other codes and, in particular, to extrapolate the plasma solution and extract fluxes of charge-exchange neutrals to the first wall and protective limiters.

Recently developed Monte-Carlo (MC) code ERO2.0 is proposed to be used to assess and predict the steady-state PWI in DEMO. ERO2.0 is a massively parallel upgrade of the original ERO code [Kir00, Kir16] that allows 3D modelling of PWI and self-consistent global impurity transport in the entire volume of a reactor-scale device, using a realistic description of all relevant PFC (e.g. based on CAD models), with a high level of local geometry resolution, and a dynamic model for microscopic morphology effects, such as surface roughness [Eks19]. ERO2.0 was designed for high-performance computing (HPC) and shows excellent parallel scaling on more than 1000 CPU cores [Rom17]. 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. The most actual reflection and erosion yields based on the Eckstein fitting formulae and Molecular Dynamics (MD) simulations are used in the code, as well as recommended atomic and molecular data from ADAS. Therefore, in particular, effects such as prompt re-deposition of heavy ions like W can be accounted for [Kir16]. 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 [Rom19a] and applied to WEST [Gal20] and ITER [Rom19b].

The electric field in front of PFC surfaces is an important factor in impurity modelling since it has direct influence on the amount of the eroded material and near-surface transport of ions, and thus on the resulting re-deposition of eroded species. Self-consistent calculations of the electric field are possible with Particle-in-Cell (PIC) codes, among which the BIT [Tsk08, Tsk17, Tsk19] and SPICE [Kom13, Kom17] code families represent the state-of-the-art. PIC codes also deliver ion fluxes and spatially resolved plasma parameters in the vicinity of surfaces, thus providing valuable analysis of other important properties like the plasma flow velocity and plasma density within the sheath [Sta12]. This information will be used to validate and improve the models for the sheath potential and plasma parameters in ERO simulations [Kir18].

The unique feature of the BIT code family (1D, 2D, 3D PIC-MC codes) is the capability to simulate neutral and impurity dynamics in the SOL, including their non-linear interaction, which makes it applicable for simulation of high recycling divertor plasma sheath [Tsk17]. In particular for DEMO, due to extremely high density divertor plasma and respective sheath collisionality characteristics, some new features of the sheath (compared to classical models) will have to be taken into account for estimation of particle and energy fluxes to the divertor plates. These are, namely, an increased broadening of the ion angular and energy distribution functions at divertor plates, and an increased sheath heat transmission factor due to super-thermal electrons originating from the upstream SOL [Tsk17]. Codes of the BIT family are massively parallel and optimized, and therefore well-suited for applications on HPC systems. Fully kinetic modelling of the DEMO divertor plasma under different conditions will provide the ERO2.0 code with the corresponding plasma profiles and necessary boundary conditions at the plasma sheath.

SPICE2 and SPICE3 are parallel PIC codes for sheath modelling that scale up to 100 cores and allow simulating wall surfaces of sophisticated geometries in 2D and 3D, respectively. SPICE codes were successfully applied to analysis of plasma behavior in the vicinity of an ion sensitive probe [Kom10] and near and inside gaps of castellated PFC [Kom13, Kom17]. PIC simulations

of plasma penetration into gaps of castellated divertor surfaces and sacrificial limiters in DEMO will allow calculating heat loads onto edges of monoblocks and impurity and fuel accumulation between them. SPICE simulations will be also used to address the effects of local electric fields at rough technical surfaces and near PWI-modified morphology on the angular distribution of impacting ions. One further feature of SPICE codes is precise simulation of thermionic emission currents from PFC [Kom20], which is crucial for modelling of W melting during transient events as will be detailed in the next section.

Provided that particle fluxes and their differential distributions at various locations at divertor plates and limiter surfaces are known and available in ERO from sheath models and PIC simulations, the actual erosion-deposition rates and surface composition dynamics are governed by collision cascades caused by energetic plasma neutrals and ions in PFC material surfaces. These collision cascades can be simulated with TRIM-line codes, such as SDTrimSP [Mut19, Hof14], based on the binary collisions approximation (BCA), and are strongly dependent on material composition. For low impact energies, typically below 100 eV, at which BCA is only conditionally applicable, Molecular Dynamics (MD) approach is often used [Las12, Mar17, Gra20], which can also account for chemical effects [Bjö13, Nor11]. The outcome of BCA and MD simulations is reduced to a PWI database of integral and differential reflection and sputtering yields. For a reliable estimation of the divertor lifetime, the respective PWI database has to cover the full range of expected parameters in terms of impact angles and energies, surface morphology, material combinations and possible chemical interactions between them. In particular, the effect of super-saturation of near-surface layer of W with hydrogen isotopes [Gao17] on W erosion yields remains an open question.

In order to provide ERO simulations with DEMO-relevant W erosion yields, including molecular sputtering yields, an extensive set of MD simulations will be performed for W under D/T super-saturation conditions. Existing W-H interatomic potentials that were proven to work well for PWI with W will be used for this task. Further effort will be put on development of W-O and W-O-H interatomic potentials that will be able to provide necessary input for ERO simulations under DEMO conditions when surfaces have been oxidized, e.g. as a result of off-normal transient events.

The MC codes of the SDTrimSP-family (1D, 2D, and 3D) have been validated multiple times and thus provide a reliable PWI database basis for predicting the wall lifetime and morphology changes. The codes are highly parallelized so that HPC-usage is rather straightforward. In order to account for erosion of rough technical W surfaces and PWI-modified W morphology, a recently developed [Tus17] and validated [Arr19] 3D version of the code is proposed to be used in combination with PIC and ERO simulations. Self-consistent coupling of 1D and 3D versions of SDTrimSP with ERO is foreseen for the second phase of the project. In addition, the SDTrimSP-3D code capabilities will be expanded with an improved in-code handling of gyro-motion of charged particles, thus enabling multifaceted approach to wall lifetime predictions and, noteworthy, implementation of uncertainly quantification (UQ) infrastructure and respective studies [Pre19].

The last but not least objective for predicting steady state PWI in DEMO is an assessment of the in-vessel tritium inventory, which will be driven by two essentially different processes. Based on JET experience [Bre13] and ITER predictions [Sch15a], the dominant retention mechanism will be co-deposition. In the case of a full-W DEMO, tritium co-deposition with W can be assessed by means of ERO simulations, where T and W transport in the SOL can be addressed self-consistently. Regions of net deposition will be identified and tritium uptake in the co-deposited layers will be calculated based on available empirical formulae [Tem09] and

models [Kra20]. Location maps of preferential deposition will in turn serve as input for dust mobilization and transport simulations described in the next section.

The second pathway for tritium inventory is retention in the bulk of PFC materials, driven by ion implantation, diffusion from plasma-exposed surfaces to underlying structures and trapping at ion- and neutron-induced defects. Burning plasma in DEMO imposes two challenges in modelling of tritium inventory by implantation, namely He-induced defects and surface modifications, localized mostly within few micrometers of the surface layer, and n-induced damage distributed through the entire bulk of PFC. Due to multi-material structure of PFC in DEMO (W armor, steels as interlayers, substrate and structural materials, CuCrZr heat sinks and Cu interlayers), modelling capabilities have to be enhanced with proper models for description of material interfaces, both in terms of temperature distribution profiles and in terms of different susceptibility to hydrogen isotopes.

The problem of fuel retention is usually tackled by macroscopic rate equations models that, compared to MD and Kinetic Monte-Carlo, offer the possibility of simulations on much larger spatial and time scales. Thus it is possible to cover the entire PFC thickness (cm scale) and lifetime (days and years of plasma operation), still resolving fast and local processes within the implantation range of plasma ions. The proposed approach to tritium transport and retention modelling for PFC is to benefit from advancements in reaction-diffusion modelling with a group of codes developed by team member organizations in the recent years. These codes are TESSIM-X [Sch15b], CRDS [Mat18], MHIMS [Hod17], FESTIM [Del19], ABAQUS solution [Ben18], and RAVETIME [Tou21], thus offering the potential of thorough cross-validation, evaluation of crucial parameters and processes, as well as uncertainty quantification.

The code TESSIM-X has been developed to model the transport of hydrogen in defect rich materials and across material interfaces. As part of the work in WP-PFC SP3 it was validated against experimental data and was benchmarked against other codes like TMAP7 or MHIMS. It is therefore ideally suited to model retention and permeation through the DEMO first wall. CRDS can address defect mobility and damage annealing. MHIMS includes an empirical rate equation model for stabilization of displacement damage by hydrogen atoms, which can serve as a basis for modelling of retention enhancement as a function of neutron damage. MHIMS has been successfully applied to describe experiments with self-damaged W. The above codes are essentially 1D and therefore cannot be straightforwardly applied to the macroscopic monoblock geometry foreseen for DEMO protective limiters and divertor [Viz20, Mav18]. FESTIM code is built upon MHIMS, but is based on the finite element method offering the possibility of arbitrary simulation domains. It is therefore capable of 2D and 3D simulations of realistic monoblock geometries with material interfaces. The interface model of FESTIM is being currently finalized and validated with application aiming at ITER divertor monoblocks. FESTIM simulations are supported by standalone FEM simulations in ABAQUS aiming at thermomechanical coupling for realistic description of influence of He-clustering on hydrogen retention and transport. There is a strong link with several WP PWIE activities, which will significantly improve the fundamental knowledge base regarding hydrogen interactions, in particular, with He- and n-induced defects.

To achieve predictive capabilities, it is of great importance to study the effects of uncertainty on the simulation result. RAVETIME is a parallel finite-volume 3D transport code designed to take advantage of developments within the European Exascale computing project VECMA on UQ methods. For given uncertainties in input parameters, RAVETIME can compute the uncertainty of hydrogen uptake in W and permeation through W armor layer and across material interfaces. As a part of the TSVV task, the code will be augmented to include fusion specific

processes and validated against TESSIM-X and others. For UQ purposes for DEMO, RAVETIME will be executed massively parallel on HPC systems.

3. Approach to PWI during transient events

The envisaged main plasma transients in DEMO are the regular rump-up phases, upward and downward vertical displacement events (VDE) and the loss of confinement (H-L transition) [Viz20]. In order to protect the first wall, several limiters are proposed to be installed at different specific locations in the plasma chamber [Mav20, Viz20]. Erosion, in particular by melting and melt splashing, is of concern. In the recent years the KTH group has developed and validated a set of numerical tools for modelling of macroscopic melt motion, non-linear surface deformations and melt splashing, as well as dust/droplet transport, in-vessel survival and accumulation.

The study of melt events induced by transient heat and current loads requires the treatment of free-surface magneto-hydrodynamic flows with phase transitions. These are fundamentally multi-scale phenomena: the motion of molten material along PFC with characteristic distances of 1-10 cm over a few tens of milliseconds, the melt depth typically of the order of 100 µm, and nonlinear free-surface instabilities, eventually responsible for splashing, developing on much smaller spatiotemporal scales. Fully self-consistent numerical models are generally considered too computationally expensive. The problem can be approached by combining the MEMOS-U code [Tho18, Rat20] with customized ANSYS set-ups.

MEMOS-U solves the incompressible resistive thermoelectric magneto-hydrodynamic equations in the magneto-static limit, together with the heat convection-diffusion equation [Tho18, Rat20]. It utilizes the shallow water approximation that drastically decreases computational costs. MEMOS-U is parallelized and runs on IO clusters. The role of thermionic emission is crucial in modelling W melting events and the MEMOS-U description of the escaping thermionic current is based on the state-of-the-art PIC modelling of strongly emissive magnetized sheaths with the SPICE code [Kom20] introduced in the previous section. As validation against experiments revealed [Rat20], MEMOS-U is well suited for predicting the macroscopic PFC response to transient heat loads: large wetted areas, long heat load durations and bulk motion of shallow liquid metal pools. In the frame of the project, the geometry of molten PFC will be exported into ERO and SDTrimSP-3D to evaluate the effective erosion of re-solidified melt in subsequent plasma operation.

Smaller-scale flow features such as strong free-surface deformations and melt ejection are simulated with customized set-ups in ANSYS that solve the coupled multi-phase Navier-Stokes and heat equations using the volume-of-fluid method, with plasma heat and momentum drive as boundary conditions. Large-scale characteristic of the flow predicted by MEMOS-U (e.g. nominal melt depth and velocity profile) are enforced via appropriate boundary conditions. Such modelling allows establishing a catalogue of representative scenarios corresponding to various models of dust/droplet production.

In addition to droplet ejection during transient melt events, also destabilization of deposited layers can serve as a source of mobilizable dust in the reactor. Re-mobilization of pre-existing dust under steady state and transient plasma conditions is another directly related issue [Rat17]. The dynamics of heavy W dust is largely inertial thus initial release conditions play a pivotal role in predicting the lifetime and final in-vessel locations of particles. The release conditions for mobilizable dust are dictated by the adhesive dust-wall contact, whose modelling was tested in multiple linear generators as part of past WP PFC activity by the KTH group. Empirical scaling laws are available and will be used to formulate initial conditions for dust speed and size. Release locations can be determined from areas of efficient net deposition identified by

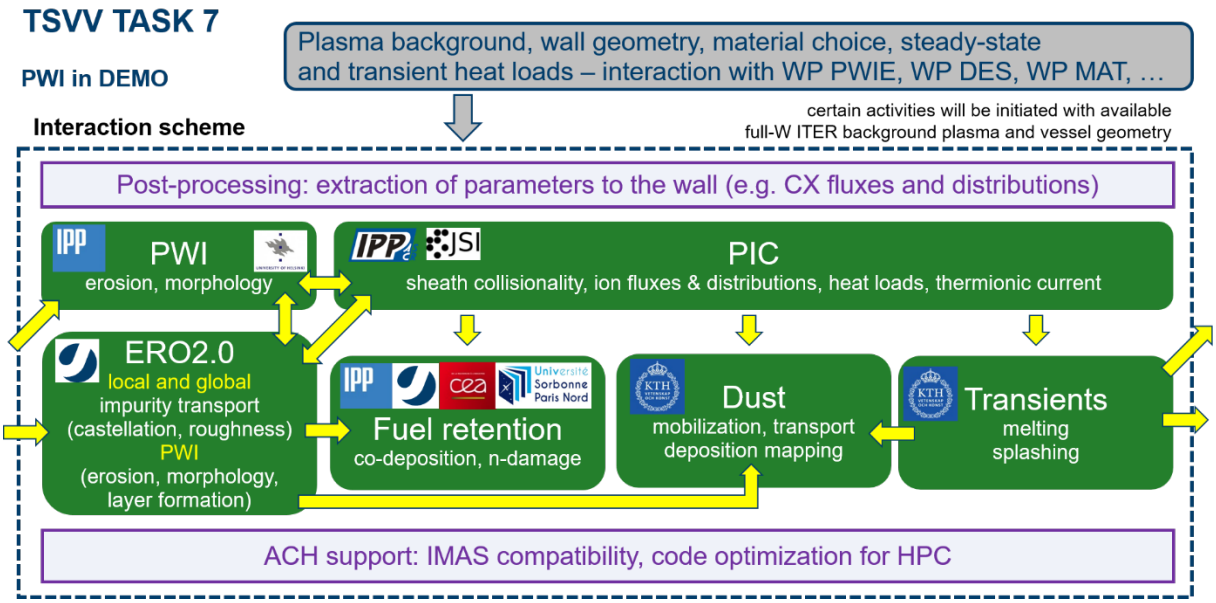
ERO modelling, as well as from in-vessel accumulation maps of previously traced droplets produced during transient melt events.

The MIGRAINe code [Vig14, Vig17, Vig18a] incorporates state-of-the-art models for numerous physical processes governing the heating and lifetime of metallic dust and droplets in full 3D environments relevant to ITER and DEMO (e.g. CAD based geometry). The code solves a coupled system of equations describing the charging, heating, motion and mass ablation of spherical particles immersed in a prescribed plasma environment (e.g. start-up, steady-state or disrupting plasmas), and features a comprehensive description of in-vessel dust migration due to collisions with PFC, based on contact mechanics models. The output of multiple single-trajectory simulations for varying initial conditions can be combined to extract quantities of practical interest, such as the overall dust survival rate, and the size distribution and spatial deposition patterns of mobilizable dust on the vessel wall. MIGRAINe simulations relating to long-distance dust migration in tokamaks and dust survivability in divertor-like plasmas have been successfully validated against in situ dust injection experiments [Rat13, Vig18b].

It is important to highlight that, as for steady state PWI, wall geometry, material choices and plasma profiles represent crucial external input for modelling of PWI caused by transients. To model the PFC response to transient heat loads using MEMOS-U, the surface heat fluxes during DEMO VDEs and loss of confinement events have to be provided, along with the halo current density for current quench scenarios. Ideally, this implies spatiotemporal profiles [Cob20], but in case when such input is not readily available, representative values of these quantities along with the event duration and wetted area estimates can be used for initial evaluations. For MIGRAINe modelling of droplet survival in disrupting plasmas, the input consists of time-evolving profiles of plasma temperature and density, including impurity and mitigating species [Vig18a]. Profiles based on simplifying assumptions concerning spatial and temporal evolution can be used for an initial evaluation of droplet survival rates and accumulation sites. In all cases, respective input from related work packages is essential.

4. Interaction scheme for PWI modelling

The scheme below summarizes the integrated approach to PWI modelling for DEMO. Each block represents a subtask. Subtasks are linked by boundary conditions and data exchange.



5. Milestones

Year 1: ITER-like plasma case

M1.1	SOLPS-ITER steady-state plasma background (ITER plasma) is adapted to DEMO, post-processed for ERO2.0 and MIGRAINe, relevant data are extracted for PIC simulations.
M1.2	Scoping PIC simulations are performed to assess the characteristics of the plasma sheath and resulting impact angles and energies in steady state.
M1.3	Intermediate results on erosion of H supersaturated W from MD simulations are reported.
M1.4	MIGRAINe scoping dust transport simulations with ITER-like ramp-up and steady state plasma profiles are performed.
M1.5	Thermo-migration is implemented in TESSIM-X and validated.
M1.6	Validation of the interface model of FESTIM is completed.
M1.7	Common test cases for retention modelling are identified.
M1.8	HPC optimization requirements for the codes are identified, the respective work initiated.

Year 2: SOLPS DEMO solution

M2.1	Preliminary ERO2.0 simulations with existing PWI database, sheath models and adapted ITER-like plasma background are performed, first erosion-deposition maps are provided.
M2.2	MIGRAINe dust transport simulations are performed using ITER-like profiles and preferable net deposition locations provided by preliminary ERO2.0 runs.
M2.3	DEMO plasma background is obtained (external input from relevant work packages), post-processed to be used in ERO2.0 and MIGRAINe, relevant data for PIC are extracted.
M2.4	Scoping PIC simulations including combined thermionic emission and secondary electron emission are performed, validity of existing scalings for MEMOS-U simulations assessed.
M2.5	Final results on erosion of D/T supersaturated W from MD simulations are reported.
M2.6	Representative values of surface heat fluxes and halo current densities during DEMO VDEs and surface heat fluxes during DEMO loss of confinement events are obtained (external input). The respective data are processed for MEMOS-U simulations.
M2.7	Gyromotion module is implemented in SDTrimSP-3D.
M2.8	Neutron damage model with damage stabilization is implemented in FESTIM and TESSIM-X (validation not yet completed).
M2.9	TESSIM-X, MHIMS and FESTIM simulations of H retention under DEMO conditions (without n-damage) and relevant material structures are performed.
M2.10	IMAS compatibility requirements for the codes are detailed and the work is initiated.

Year 3: Conceptual design review

M3.1	Erosion data under DEMO D/T supersaturation is implemented in ERO2.0.
M3.2	Erosion-deposition maps from ERO2.0 with DEMO plasma solution are provided.
M3.3	MEMOS-U simulations of PFC response under VDEs and loss of confinement are performed, macroscopic surface modifications and melt splashing are assessed.
M3.4	MIGRAINe dust transport simulations are performed using DEMO steady state profiles and preferable net deposition locations provided by ERO2.0.
M3.5	SDTrimSP-3D simulations are performed to assess the role of rough surfaces and re-solidified melt morphology on effective erosion yields.
M3.6	Role of gaps between divertor and limiter monoblocks is addressed by means of PIC simulations (heat loads and ion penetration).
M3.7	TESSIM-X and FESTIM simulations of H retention under DEMO conditions (with n-damage) and relevant material structures are performed and cross-validated.
M3.8	Intermediate results on W-O potential development are reported.
M3.9	Integrated results regarding W erosion (steady state and transients) and T retention for the DEMO conceptual design review are reported.
M3.10	Intermediate results on IMAS interfaces implementation are reported.
M3.11	Transient plasma profiles representative of VDEs and loss of confinement events in DEMO are obtained (external input) and implemented in MIGRAINe.

Year 4: Extended analysis

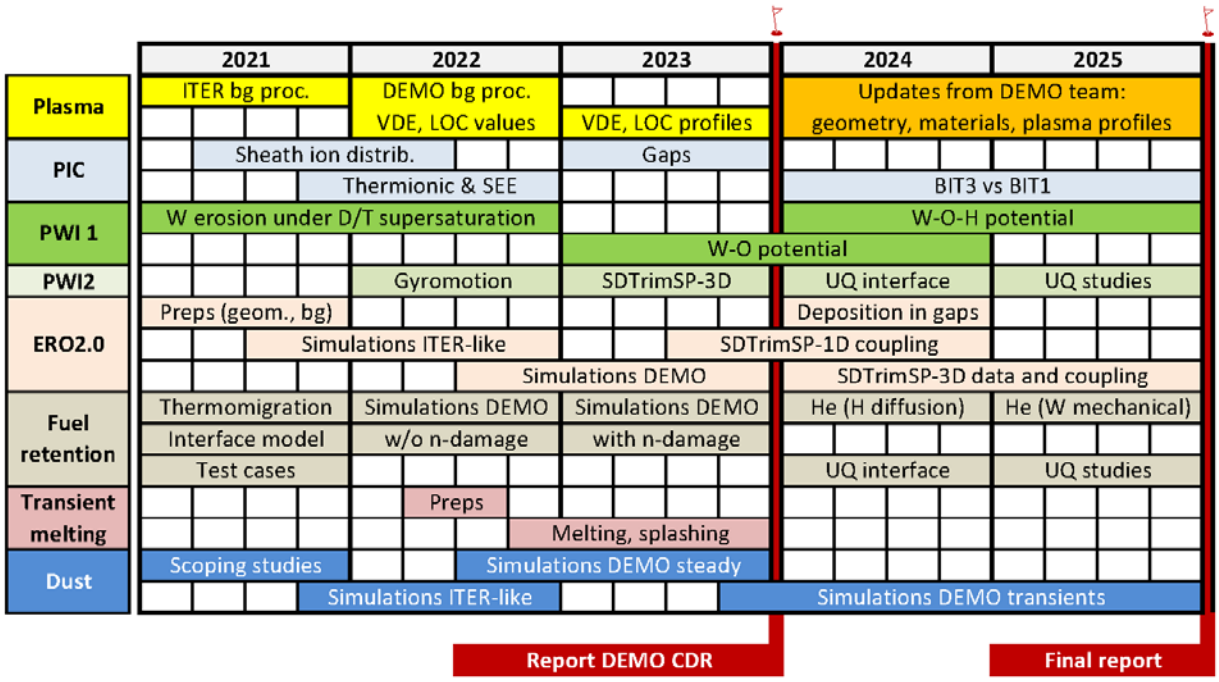
M4.1	Deposition in gaps between divertor and limiter monoblocks is assessed by ERO2.0.
M4.2	SDTrimSP-3D results regarding rough surfaces are incorporated into ERO and cross-validated on selected cases using built-in morphology model of ERO.
M4.3	SDTrimSP-1D coupling to ERO2.0 is finalized (for global scale modelling).
M4.4	Final results on W-O potential development are reported.
M4.5	Intermediate results on W-O-H potential development are reported.
M4.6	Role of He clustering on H diffusion and retention is assessed.
M4.7	Preliminary BIT3 simulations are reported (fully kinetic sheath in 3D).
M4.8	IMAS compatibility is implemented.
M4.9	UQ interface implementations for SDTrimSP codes and RAVETIME are finalized.
M4.10	MIGRAINe transport simulations are performed for droplets in DEMO plasma transients.

Year 5: Final reporting

M5.1	Final results on W-O-H potential development are reported.
M5.2	Role of He clustering on mechanical properties of W is assessed.
M5.3	BIT3 simulations are finalized and compared to 1D cases.
M5.4	SDTrimSP-3D coupling to ERO2.0 is finalized (for local scale modelling).
M5.5	UQ studies with SDTrimSP codes and with RAVETIME are performed.
M5.6	Post-processing of final MIGRAINe simulations for DEMO plasma transients is finalized.
M5.7	HPC optimization completed.
M5.8	IMAS compatibility between codes and their interfacing is complete and tested.
M5.9	Integrated results on W erosion (steady state and transients) and T retention are reported.

The list of possible extensions to the above workplan beyond the 5-year project period includes but is not limited to the following topics: assessment of He-induced surface modifications (fuzz growth, effect on erosion and lifetime), assessment of W transmutations and presence of other impurities (fuel retention), application to new or alternative geometries and plasma configurations, assessment of the feedback loop to the plasma (interaction with other TSVVs and work packages).

6. Envisaged project timeline (ACH contribution not included)



7. Deliverables

D1	Steady state W erosion rates at DEMO first wall and divertor.
D2	Location mapping for net (co-)deposition and impurity sources from the wall.
D3	Large-scale surface modifications due to melting and melt-motion induced by transients.
D4	Assessment of surface roughness and lifetime of PFC affected by transients.
D5	Stability of melt layers during transients. Droplet sizes and speeds in case of splashing.
D6	A catalog of representative cases for dust (re-)mobilization conditions.
D7	Dust survival rates, inventory evolution and accumulation maps of re-solidified droplets.
D8	Prediction of fuel inventory in multi-component PFC including thermal and mechanical effects, accounting for neutron and He damage, morphological changes.
D9	Uptake of D/T in W and across interfaces to the coolant and respective UQ.
D10	Fully kinetic sheath simulations in 1D/3D providing plasma profiles and boundary conditions at the plasma sheath based on the DEMO plasma solution.
D11	Effective W erosion yields for rough surfaces and re-solidified melt layers, including UQ.
D12	W erosion yields under D/T supersaturation as function of ion impact energies, angles, and surface temperature.
D13	W-O and W-O-H interatomic potentials.
D14	A suite of HPC optimized codes for DEMO PWI with IMAS-adapted data exchange.

8. Risk assessment

Risk	Impact	Fallback solution
SOLPS-ITER plasma solution is not available by 2022-23.	Delays in meeting milestones regarding steady state wall erosion and retention.	Evaluations will start with available ITER plasma solution(s) (full-W ITER).
DEMO transient profiles are not available during the course of the project, even in the simplified manner.	Delays in meeting milestones or milestones regarding transient melt events and dust release / transport not met.	MEMOS-U and MIGRAINe simulations with available ITER transient profiles. Their relevance to be assessed by DEMO experts.
Developing an analytical W-O potential turns out to be impossible due to very complex W-O phase diagram.	Delays in meeting respective milestones due to slower simulations in case of the fallback solution.	Gaussian Approximation Potential (GAP) machine learning formalism will be applied. This is more likely to be flexible enough, however will lead to much slower simulations.
Lack of support & poor IMAS API documentation.	Delays in implementing IMAS interfaces for most of codes involved.	ACH support will allow timely reaching the milestones regarding IMAS.
Underestimated computational effort/cost for PIC simulations (fully kinetic modelling for DEMO plasma edge never done so far).	Delay in the implementation of proper plasma parameters and boundary conditions to other codes. Delays in meeting milestones.	Evaluations will start with available databases, sheath models and boundary conditions (ITER-like). Computational efforts will be re-evaluated timely during the project.
Complex and/or small-scale PFC geometries that cannot be fairly approximated by flat surfaces are impossible to handle with MEMOS-U given the model limitations.	Maintaining reasonable computational costs will require a trade-off between spatial resolution and the overall dimensions of the simulated volume.	If MEMOS-U fails to treat such cases, the customized set-ups in ANSYS can be used instead, resulting in higher computational costs or lower spatial resolution due to essentially 3D melt dynamics.
Lack of support in HPC upscaling for uncertainty assessment tasks.	Only a small number of parameters studied, likely overconfident predictions.	ACH support will allow mitigating this risk.
Staff replacements / manpower not available.	Delays in meeting the milestones.	Research units have to ensure the staff availability and continuity.

9. List of references

[Arr19] R. Arredondo et al., Nucl. Mater. Energy 18 (2019) 72–76
[Ben18] S. Benannoune et al. Int. J. Hydrogen Energy 43 (2018) 9083-9093
[Bjö13] C Björkas et al., Plasma Phys. Control. Fusion 55 (2013) 074004
[Bre13] S. Brezinsek, T. Loarer, V. Philipps, et al., Nucl. Fusion 53 (2013) 083023
[Cob20] J. Coburn *et al*, *Phys. Scr.* T171 (2020) 014076
[Del20] R. Delaporte-Mathurin et al., Nucl. Mater. Energy 21 (2019) 100709
[Eks19] A. Eksaeva et al., Nucl. Mater. Energy 19 (2019) 13-18
[Gal20] A. Gallo et al., Phys. Scr. T171 (2020) 014013
[Gao17] L. Gao et al., Nucl. Fusion 57 (2017) 016026
[Gra20] F. Granberg et al., J. Nucl. Mater. 529 (2020) 016026
[Hod17] E.A. Hodille et al., Nucl. Fusion 57 (2017) 056002
[Hof14] H. Hofsäss et al., Applied Surface Science 310 (2014) 134–141
[Kav20] E. Kaveeva et al., Nucl. Fusion 60 (2020) 046019
[Kir00] A. Kirschner et al., Nucl. Fusion 40 (2000) 989
[Kir16] A. Kirschner et al., Contrib. to Plasma Phys. 56 (2016) 622–627
[Kir18] A. Kirschner et al., Plasma Phys. Control. Fusion 60 (2018) 014041
[Kom10] M. Komm et al., Plasma Phys. Control. Fusion 53 (2011) 015005
[Kom13] M. Komm et al., Plasma Phys. Control. Fusion 55 (2013) 025006
[Kom17] M. Komm et al., Nucl. Fusion 57 (2017) 126047
[Kom20] M. Komm et al., Nucl. Fusion 60 (2020) 054002
[Kra20] S. Krat et al., Nucl. Mater. Energy 24 (2020) 100763
[Las12] A. Lasa et al., J. Nucl. Mater. 429 (2012) 284–292
[Mar17] E. Marenkov et al., J. Nucl. Mater. 496 (2017) 18-23
[Mat18] D. Matveev et al., Nucl. Instrum. Methods. Phys. Res. B. 430 (2018) 23-30
[Mav18] F. Maviglia et al., Fus. Eng. Design 136 (2018) 1322–1326
[Mav20] F. Maviglia et al., Fus. Eng. Design, 158 (2020) 111713
[Mut19] A. Mutzke et al., Max-Planck-Institut für Plasmaphysik (2019) IPP-2019-02
[Nor11] K. Nordlund et al., Nucl. Instr. Meth. Phys. Res. B 269 (2011) 1257
[Pre19] R. Preuss et al., Entropy 21 (2019) 1175
[Rat13] S. Ratynskaia et al., Nucl. Fusion 53 (2013) 123002
[Rat17] S. Ratynskaia et al., Nucl. Mater. Energy 12 (2017) 569–574
[Rat20] S. Ratynskaia et al., Nucl. Fusion (2020) in press, doi: 10.1088/1741-4326/abadac
[Rom17] J. Romazanov et al., Phys. Scr. T170 (2017) 014018
[Rom19a] J. Romazanov et al., Nucl. Mater. Energy 18 (2019) 331-338
[Rom19b] J. Romazanov et al., Contrib. Plasma Phys. (2019) e201900149
[Sch15a] K. Schmid, K. Krieger, S.W. Lisgo, et al., J. Nucl. Math. 463 (2015) 66-72
[Sch15b] K. Schmid et al. J. Appl. Phys. 116 (2015) 134901
[Sta12] P.C. Stangeby, Nucl. Fusion 52 (2012) 083012
[Tem09] G.D. Temmerman and R.P. Doerner, J. Nucl. Mater. 389 (2009) 479-483
[Tho18] E. Thorén et al., Nucl. Fusion 58 (2018) 106003
[Tsk08] D. Tskhakaya et al., Contrib. Plasma Phys. 48 (2008) 121-125
[Tsk15] D. Tskhakaya et al., J. Nucl. Mater. 463 (2015) 624-628
[Tsk17] D. Tskhakaya, Plasma Phys. Control. Fusion 59 (2017) 114001
[Tsk19] D. Tskhakaya, final report of the FWF project P26544-N27, July 2019, Innsbruck
[Tou17] U. von Toussaint et al., Phys. Scr. T170 (2017) 014056
[Tou21] U. von Toussaint et al., Conf. on Bayesian Inference and MaxEnt Meth 2020, Graz, (shifted to 2021 due to Corona)
[Vig14] L. Vignitchouk et al., Plasma. Phys. Control. Fusion 56 (2014) 095005
[Vig17] L. Vignitchouk et al., Plasma Phys. Control. Fusion 59 (2017) 104002
[Vig18a] L. Vignitchouk et al., Nucl. Fusion 58 (2018) 076008
[Vig18b] L. Vignitchouk et al., Plasma Phys. Control. Fusion 60 (2018) 115002
[Viz20] Z. Vizvary et al., Fus. Eng. Design 158 (2020) 111676
[Wie15] S. Wiesen et al., J. Nucl. Mater. 463 (2015) 480–484

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)*

Expected long-term requirements of HPC resources?

It has to be noted that for the development, scoping and productive runs with most of retention and PWI codes national computational resources available at participating research institutions can and will be used. High-performance simulations using HPC systems of EUROfusion infrastructure are envisaged for the codes listed in the tables below, with indication of estimated short-term and long-term requirements.

Expected usage in the early phase of the project					
Code	CPU-h per run	Number of runs	Node hours	Number of nodes	Partition
MEMOS-U	3000	10			
BIT	1×10^6	<5	160 000	48-196	A3
SPICE	2×10^4	~20			
ERO2.0	3×10^5	5 / year	31 250	256	A3
RAVETIME	3000	20		4+	(development)

Expected long-term requirements (in addition to the above)					
Code	CPU-h per run	Number of runs	Node hours	Number of nodes	Partition
MEMOS-U	3000	10			
ANSYS	3×10^5	10			
BIT	1×10^6	<5	160 000	48-196	A3
SPICE	2×10^4	~20			
ERO2.0	3×10^5	10 / year	62 500	256	A3
RAVETIME	1×10^5	100			Partly trivial parallel capability

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.

Support of Advanced Computer Hubs (ACH) is envisaged and required mainly on two levels corresponding to the following categories from the ongoing call, Ref. PMU/1740:
Cat. 1 – High Performance Computing (HPC optimization).
Cat. 2 – Integrated Modelling and Control (IMAS adaptation and integration).

The expected ACH support totals 2 ppy/y in average over 5 years of the project duration. The respective tasks can be partly fulfilled by team members, though especially the IMAS integration would require an improved IMAS API documentation and respective support by ACH. Most of codes currently have no IMAS compatibility.

Several codes such as BIT, MEMOS-U, and SDTrimSP have been already optimized for HPC. MEMOS-U, in particular, already runs on IO clusters, however would benefit from improvements of the code architecture and modularity, in particular in terms of reduction of the memory consumption. SPICE codes scale up to 100 CPU. For simulation of the DEMO sheath with Te < 10eV these codes need massive parallelization that can be performed with help of ACH. RAVETIME also needs upscaling from cluster-parallel to HPC-parallel. MIGRAINe is inherently serial, however effective parallelization is achieved by splitting the simulated trajectories into batches. Due to potentially large number of trajectories needed to achieve statistical significance for DEMO simulations, ACH support might be necessary to ensure HPC compatibility. For the task of interatomic potential development, an ACH support for optimization and GPU-enabling is desired. Also further optimization of the ERO2.0 code is under consideration. Currently available support teams from the Jülich Supercomputing Center at FZJ and from the High-Level Support Team from the EUROfusion Infrastructure Support Activity are looking into possibilities of improved parallelisation, such as e.g. compiler optimization and GPU.