



HAL
open science

Numerical tools for burning plasmas

A Mishchenko, A Biancalani, M Borchardt, A Bottino, S Briguglio, R Dumont, J Ferreira, J Graves, T Hayward-Schneider, R Kleiber, et al.

► **To cite this version:**

A Mishchenko, A Biancalani, M Borchardt, A Bottino, S Briguglio, et al.. Numerical tools for burning plasmas. *Plasma Physics and Controlled Fusion*, 2023, 65 (6), pp.064001. 10.1088/1361-6587/acce68 . hal-04248721

HAL Id: hal-04248721

<https://hal.science/hal-04248721v1>

Submitted on 20 Oct 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Numerical tools for burning plasmas

A. Mishchenko^{1*}, A. Biancalani², M. Borchardt¹, A. Bottino³,
S. Briguglio⁴, R. Dumont⁵, J. Ferreira⁶, J. P. Graves⁷,
T. Hayward-Schneider³, R. Kleiber¹, A. Könies¹, E. Lanti⁸,
Ph. Lauber³, H. Leyh¹, Z. X. Lu³, H. Lütjens⁹, B. McMillan¹⁰,
M. Campos Pinto³, E. Poli³, B. Rettino³, B. Rofman⁷,
J. N. Sama¹¹, C. Slaby¹, F. Vannini³, L. Villard⁷, G. Vlad⁴,
X. Wang³, F. Widmer^{12,3}, F. Zonca⁴

¹ Max Planck Institute for Plasma Physics, D-17491 Greifswald, Germany

² Léonard de Vinci Pôle Universitaire, Research Center, 92916 Paris La Défense, France

³ Max Planck Institute for Plasma Physics, D-85748 Garching, Germany

⁴ ENEA, C. R. Frascati, 00044 Frascati, Italy

⁵ IRFM, CEA, F-13108 Saint-Paul-lez-Durance, France

⁶ IPFN, Instituto Superior Técnico, 1049-001 Lisboa, Portugal

⁷ Swiss Plasma Center, EPFL, CH-1015 Lausanne, Switzerland

⁸ SCITAS, EPFL, CH-1015 Lausanne, Switzerland

⁹ CNRS-CPhT-IP Paris, 91128 Palaiseau cedex, France

¹⁰ University of Warwick, Coventry, CV4 7AL, UK

¹¹ Institut Jean Lamour, UMR 7198, Université de Lorraine-CNRS, Nancy, France

¹² National Institutes of Natural Sciences (NINS), IRCC, Tokyo 181-8588, Japan

E-mail: alexey.mishchenko@ipp.mpg.de

March 2021

Abstract. The software stack under development within a European coordinated effort on tools for burning plasma modelling is presented. The project is organised as a Task (TSVV Task 10) under the new E-TASC initiative (X. Litaudon et al, Plasma Phys. Contr. Fusion, **64**, 034005 (2022)). This is a continued effort within the EUROfusion inheriting from the earlier European coordination projects as well as research projects based at various European laboratories. The ongoing work of the TSVV Tasks is supported by the Advanced Computing Hubs. Major projects requiring the High Performance Computing (HPC) resources are global gyrokinetic codes and global hybrid particle-Magnetohydrodynamics (MHD) codes. Also applications using the integrated modeling tools, such as the Energetic-Particle Workflow, based on the ITER Integrated Modelling & Analysis Suite (IMAS), or the code package for modelling radio-frequency heating and fast-ion generation may require intensive computation and a substantial memory footprint. The continual development of these codes both on the physics side and on the HPC side allows us to tackle frontier problems, such as the interaction of turbulence with MHD-type modes in the presence of fast particles. One of the important mandated outcomes of the E-TASC project is the IMAS-enabling of EUROfusion codes and release of the software stack to the EUROfusion community.

Keywords: burning plasma, energetic particles, simulations

1. Introduction

The ITER baseline scenario [1] will be characterised by plasma heating dominated by fusion-born alpha particles, and a future DEMO reactor will operate close to ignition, employing auxiliary power only for control purposes. In all present devices, generation of a significant fraction of alpha particles is difficult. This makes understanding of burning plasma physics an urgent point to be addressed through theory and simulations.

In this paper, we describe numerical codes under development for burning plasmas in the scope of the EUROfusion theory and advanced simulation coordination (E-TASC) programme [2]. This development is carried out within the Theory, Simulation, Verification and Validation (TSVV) Task 10, which is a part of the E-TASC initiative dedicated to theory and simulations of burning plasmas.

The TSVV projects, including the one described here, provide an increased level of coordination. They build on achievements and continue efforts of earlier European coordinating structures, such as the EFDA Integrated Tokamak Modeling [3, 4], EUROfusion's Workpackage "Code Development" (WP-CD) [5], EUROfusion's Workpackage "Infrastructure and Support Activities" (WP-ISA), the EFDA High Level Support Team (HLST) [6], and its continuation into the EUROfusion. Also, a number of past EUROfusion's Enabling Research projects (such as "Multi-scale Energetic particle Transport in fusion devices", "Nonlinear 3D simulations of plasma core instabilities beyond MHD in tokamak plasmas", etc.) have played a fundamental role for the TSVV Task 10. Another key ingredient in the TSVV structure are the laboratory based research initiatives. For TSVV Task 10, the main contributions include the particle-in-cell code development at the Max Planck Institute for Plasma Physics (IPP) and the Swiss Federal Institute of Technology Lausanne (EPFL); nonlinear MHD and hybrid MHD codes as well as theory from the French Alternative Energies and Atomic Energy Commission (CEA), French National Centre for Scientific Research (CNRS), and Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA); reduced energetic-particle and transport modeling from IPP and the Instituto Superior Técnico of the University of Lisbon. The ongoing work at the TSVV Tasks is supported by the Advanced Computing Hubs (ACH) [2]. For the TSVV Task 10, the key contributors are the Hubs based at the EPFL and IPP (focusing on the High-Performance Computing aspects), as well as the Core Software Integration Hub at the Poznan Supercomputing and Networking Center.

Fusion alphas and energetic particles in reactor-relevant plasmas have a unique and crucial role as mediators of cross-scale couplings [7, 8]. This makes transport in fusion devices a multi-spatiotemporal-scale process and introduces a coupling of various physical subsystems which cannot anymore be considered as isolated parts. A complicating factor here is that the physics interactions mediated by the energetic particles are volumetric rather than through simple local interfaces which makes the scale

separation more complex (or impossible) compared to the most other areas of research. As a consequence, predictive analyses based on first principles computations becomes very challenging. Developing a detailed understanding of such complex nonlinear dynamics in fusion-reactor plasmas in both tokamak and stellarator geometries is essential. In our TSVV Task “Physics of Burning Plasmas” (TSVV Task 10), we address the following subsystems of burning plasma physics:

- (i) turbulence, turbulent structures (zonal flows, avalanches, profile corrugations), and transport
- (ii) energetic particles and Alfvénic modes; phase-space structures (holes, clumps, auto-resonant “chirping” dynamics)
- (iii) MHD stability and profile evolution (sawteeth, tearing instabilities).

In our project, we focus on the core-plasma dynamics since it is the core of the plasma which is expected to burn. For the subsystem coupling, we note the following examples.

- (i) Turbulence leads to anomalous transport but it is affected by emergent structures such as zonal flows and avalanches. Energetic particles can destabilize Alfvénic modes and be transported by these instabilities.
- (ii) The nonlinear dynamics of destabilized Alfvén Eigenmodes may result in a zonal flow generation [9, 10] which can affect (e. g. stabilize [11]) turbulence.
- (iii) MHD phenomena, such as sawteeth may lead to strong particle redistribution (for the both bulk-plasma and energetic species) and hence affect the Alfvénic dynamics and fusion. On the other hand, the sawteeth can be affected by the energetic particles playing a stabilizing role on the underlying instabilities but also leading to the appearance of particularly strong “monster” sawteeth [12].

Strong coupling between different subsystems of fusion plasma dynamics calls for a unified framework which includes all these pieces self-consistently on the same footing. Many features of the subsystems relevant for the core burning plasma are kinetic and global, and many links between these subsystems are kinetic and global, too. This implies that the global gyrokinetic method is the minimal inclusive approach which may take into account the relevant complexity and mutual dependencies. Note that the items in the list above are not exclusive. One aspect, not included in the list, concerns global kinetic turbulence self-organization, e. g. the transport barrier formation [13], with a strong profile evolution coupled to the neoclassical physics and controlled by the particle and energy sources. This kind of physics will be affected by the energetic ions in burning plasmas and shall be addressed using flux-driven full-f codes such as GYSELA [14]. Presently, GYSELA is not a part of the TSVV Task 10 program. Up to now, this code has mainly been used in the electrostatic regime.

In our project, we employ the global electromagnetic gyrokinetic codes ORB5 [15, 16] and EUTERPE [17] which can be used in tokamak and stellarator (in the case of EUTERPE) geometries. Using these gyrokinetic codes, we study electromagnetic turbulence in different regimes [18, 19, 20, 21], consider meso-scale couplings of the

turbulent dynamics to the MHD-like tearing and kink modes [21], and study interaction with the Alfvénic instabilities in the presence of energetic ions [22, 23, 24, 25, 26, 27, 28]. Note that ORB5 and EUTERPE are included in other TSVV Tasks as well. In our Task, the focus is on the electromagnetic applications of these codes.

Global gyrokinetic simulations are very expensive and time consuming. Therefore, developing reduced models, supporting and supported by the first-principle simulations, is indispensable. There are different degrees of reduction possible. To consider the nonlinear MHD time scale, such as the sawtooth cycle or a fishbone burst, a hybrid MHD approach can be used. Here, the energetic-particle dynamics is considered using the full-kinetic or the gyrokinetic method whereas the bulk plasma is described solving the MHD equations. For this purpose, we use the nonlinear-MHD code XTOR-K [29, 30, 31], which solves the full kinetic problem for the energetic particles. Using XTOR-K, the sawtooth dynamics can be considered in the presence of energetic ions. The latter can modify the stability properties of the precursor internal kink instability but can also be transported by the sawteeth, altering their couplings to the Alfvénic continuum and Eigenmodes, as it has been seen in recent JET experiments [32].

Also fishbones or energetic particle modes may lead to a non-diffusive transport of energetic particles [8, 33]. In burning plasmas it can strongly affect the fusion reactivity and the overall system performance. For these instabilities, the main nonlinearity is on the energetic particles whereas the bulk plasma can be described with a good accuracy solving the linear full MHD equations, i. e. neglecting the wave-wave nonlinearity. This approach is realized in the HYMAGYC code [34] whereas the HMGC code [35] solves the nonlinear reduced-MHD equations to describe the bulk plasma. In stellarator geometry, the hybrid particle-MHD code CKA-EUTERPE [36] is used. An important feature of HYMAGYC is its almost complete IMAS-enabling based on a machine-generic data dictionary [37]. IMAS (ITER Integrated Modelling and Analysis Suite [37]) is a key standardization tool for E-TASC and EUROfusion data and code integration [2] based on the physics Data Dictionary and the Interface Data Structures (IDS) [37] typically describing tokamak subsystems (such as equilibrium or heating). HYMAGYC can be run as an embedded IMAS actor [37] in an integrated environment. New IDS structures have been identified during the IMAS-enabling of HYMAGYC which should be included in the next IMAS releases. These new IDS structures can be used in future by other energetic particle and MHD stability codes. Note that most of the codes developed within the TSVV Task 10 implement unified interfaces based on the IDS structures. One exception is EUTERPE where IDS interface implementation is complicated by the stellarator geometry (IMAS is focused on tokamak applications).

Hybrid-MHD simulations are more affordable than the full gyrokinetic approach but they can also become prohibitively expensive on the full discharge time scale. Here, integrated modelling based on the IDS coupling of several codes becomes the only possible approach. The key part of this setup, further developed in our project, is the new Energetic-Particle Workflow. It is a pythonic framework which couples equilibrium codes, such as the CHEASE [38] or HELENA [39], transport codes, such as the ETS

[40], heating codes (e. g. NUBEAM [41]), and the LIGKA-HAGIS codes [42, 43] which describe the nonlinear fast-ion dynamics on a short time scale. The resulting energetic-particle distribution function can be used on the next time step to advance the plasma profiles and the equilibrium, if needed. To speed-up the computations, pre-calculated phase-space zonals structures for a set of Alfvénic modes at fixed amplitudes (somewhat similar to the kick-model approach of Ref. [44]) can be employed to calculate phase-space dependent energetic-particle diffusion coefficients which can be used in the heating codes.

The new Energetic-Particle Workflow has only been developed for tokamaks so far. In future, this framework will be extended to stellarator geometries using the CONTI code [45] and the CKA-EUTERPE code [36] as the main ingredients. The CONTI code computes shear Alfvén continua in general toroidal geometry based on a VMEC [46] equilibrium. The CKA-EUTERPE code can be used to study the nonlinear energetic-particle dynamics in stellarator geometry interacting with a prescribed set of Alfvén Eigenmodes. In future, these tools can be combined in an automated manner resulting in a similar workflow for stellarators.

Although most of the heating in a burning plasma should be provided by fusion-born alpha particles, auxiliary heating will still be of importance before the plasma ignition is achieved and also later for discharge control. In our project, we employ the SCENIC framework [47], which describes ICRH plasma heating and energetic-ion generation via a combination of three codes: LEMan [48] solving the hot-plasma wave-propagation equations, VENUS-LEVIS [49] tracing energetic-particle orbits and using Monte Carlo kick operators [50] for collisions and interaction with the wave field, and ANIMEC [51] solving for a plasma equilibrium with an anisotropic energetic-ion pressure tensor. The role of SCENIC in the TSVV Task 10 is to provide an energetic-particle distribution function needed as input by the stability codes.

In summary, our codes are employed to provide a self-consistent description of the mutual interaction of energetic particles with MHD modes and turbulence, as well as their interplay with the kinetic plasma profiles in both tokamak and stellarator geometries. In future, they will be used to develop strategies optimizing deposition of the fusion alpha energy to the bulk plasma and improving the reactor performance.

This paper is organized as follows. In Section 2 we detail the description of the codes developed by the TSVV Task 10 and address the main simulation results. In Section 3, we summarize our conclusions.

2. Software stack of TSVV Task “Physics of Burning Plasmas”

2.1. Gyrokinetic codes

ORB5 and EUTERPE are global codes solving the nonlinear electromagnetic gyrokinetic Vlasov-Maxwell system of equations [52] in tokamak and stellarator geometries using a particle-in-cell (PIC) scheme. The codes assume multiple gyrokinetic ion species and drift-kinetic electrons. The choice of the ion species mix is completely general

and can include energetic ions (e. g. alpha particles), impurities (Ar, Be, etc.), isotope fuels (Deuterium and Tritium), or Helium ash. The same freedom of choice applies also for the leptonic component. For example, ORB5 has been used to simulate electron-positron pair plasmas [53]. All the species are treated on the same footing. The gyrokinetic ions imply that the codes can be used at all wavelengths ranging from the global to the ion gyro-radius scale and below. Several types of collision operators are available in the codes ranging from a simple Lorentz collision operator [54] to more general operators based on the Rosenbluth potentials [55]. A Fourier filter in the toroidal and poloidal directions as well as various control variates and noise reduction techniques [15] enable simulations with good signal-to-noise ratio at a limited numerical cost. For electromagnetic simulations, the control-variate and the pullback mitigation techniques [56, 57] are available. As a subset, ORB5 and EUTERPE include fluid-electron and fluid-bulk kinetic-energetic-particle models [58] as well as the CKA-EUTERPE model [36]. ORB5 runs on both CPUs and GPUs [16]. EUTERPE has been extended to GPUs recently. Code testing in a production environment is ongoing. The codes are well benchmarked [59, 60, 61, 62, 63] against other similar codes and analytical predictions and show good scalability (see Refs. [15, 16, 64] addressing the performance of the codes on many- and multi-core architectures). EUTERPE is specialized for simulations in three-dimensional (stellarator) geometry using a plasma equilibrium calculated with the VMEC [46] or GVEC [65] codes. Two coordinate systems are used in EUTERPE: a system of magnetic coordinates (PEST) for the field solver and cylindrical coordinates for the equilibrium and to push the particles. The magnetic coordinate system employed for the field solver facilitates handling of complex shaped geometries, typical for stellarator plasmas. The change between the coordinate systems is done using linear interpolation. The quality of the interpolation (the corresponding grid size) should be good enough for a numerical accuracy of the codes. However, the interpolation is needed in the real space only and appears to be less problematic than in semi-Lagrangian codes [66] where the distribution function has to be interpolated in the phase space. The equations for the perturbed field are solved using the PETSc [67] library. The integration of the Vlasov equation is usually done using an explicit fourth order Runge-Kutta scheme. ORB5 can use realistic CHEASE [38] equilibrium.

Global gyrokinetic simulations of electromagnetic turbulence have been performed using ORB5 and EUTERPE in presence of energetic particles and global MHD-like (tearing) modes at different beta values in realistically shaped tokamak and stellarator geometries [20, 21]. A transition from electromagnetic ITG to KBM regimes has been observed in ASDEX-Upgrade and ITER using ORB5. For stellarators, such a transition between the different turbulence regimes has been considered using EUTERPE in various configurations of W7-X as well as new optimized stellarator geometries. First ORB5 results (TAE modes) are available for JET plasmas, see Fig. [1] for an example. Non-adiabatic chirping dynamics of TAEs and EPs has been studied [69] using HMGC (non-perturbative hybrid particle-MHD approach) and ORB5 (fully gyrokinetic for all particle species, including the electrons). The results compare well to each other and

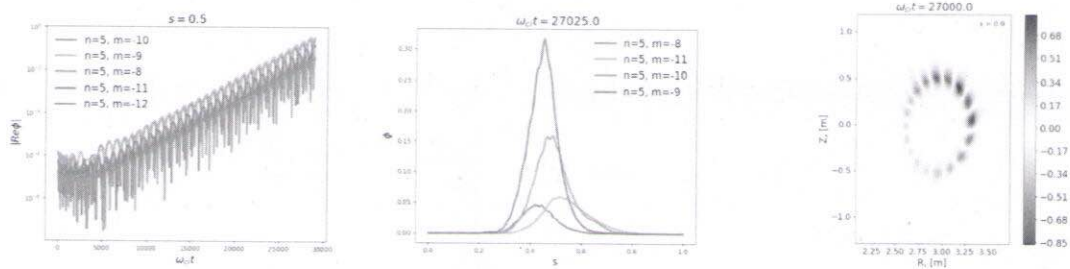


Figure 1. Evolution and mode structure of the TAE instability for JET (configuration as in Ref. [68]). The mode frequency obtained with ORB5 is $\omega/\omega_A \approx 0.27$. The Fourier filter employed in this simulation corresponds to a single toroidal mode $n = 5$ and 11 poloidal modes $5 \leq m \leq 15$.

demonstrate numerically the importance of the “Trap-Release-Amplify” mechanism [70] for the phase-space evolution of chirping instabilities. This mechanism has been studied analytically [71] both in the context of burning fusion and space plasmas, where a similar theoretical framework based on the Schwinger-Dyson equation can be applied to describe the evolution of phase space zonal structures [8, 33]. These structures can be understood as the evolution of the system through neighboring nonlinear equilibria [72]. The Hamiltonian-mapping diagnostics has been applied in HMGC to study the phase-space dynamics of the particles in the chirping modes which have also been studied with the fully gyrokinetic EUTERPE and the reduced CKA-EUTERPE model [36]. For ORB5, a dedicated finite element representation of phase space zonal structures has been introduced [73] which can be used for various purposes, including chirping dynamics. Fully numerical energetic-particle distribution functions (e. g. generated by the NBI) have been applied in ORB5 [25]. Validation of ORB5 using realistic distribution functions for ASDEX-Upgrade discharge #31213 has been extended to the nonlinear regime [24]. It has been shown that realistic energetic-particle distribution functions are essential to reproduce quantitatively the experimental results. Multi-scale analysis of global electromagnetic instabilities has been carried out using ORB5 in ITER Pre-Fusion Power Operation (PFPO) plasmas as a part of an international effort under the EP-ITPA umbrella [27]. It has been shown that Alfvénic instabilities can be excited by the thermal ions in ITER plasmas even in the absence of energetic ions providing the toroidal mode numbers are high enough [27].

2.2. Hybrid particle-MHD approach

XTOR-K solves nonlinear 3D extended MHD equations coupled self-consistently with a full-f full-orbit or guiding center PIC time advance for selected populations of kinetic particles. The implicit fluid part in the time advance is inverted using a pre-conditioned matrix-free GMRES solver [29]. A substantial effort has been undertaken in the last two years to parallelize the inversion of the physical pre-conditioner using a SPIKE LU

solver which solved the problem of small time steps in the saturated kink regime. It has resulted in an overall factor 2.5 speed-up of the code. Another factor 2 speed-up has been achieved due to particle sorting which strongly reduces cache missing for moment depositions. Successful simulations have been performed for the TAE mode destabilized by the energetic particles (the “ITPA benchmark” [74, 75]). For a correct simulation of sawtooth oscillations, the model in the fluid part of the code had to be improved and benchmarked from resistive MHD (used in previously done fishbone studies [31,]) to a more general two-fluid model. The model differs from the one in the old two-fluid MHD XTOR-2F because bulk ion and electron temperatures evolve separately in XTOR-K. Also, the components of the MHD equations parallel and perpendicular to the magnetic field are treated differently. All these physical model and performance improvements were necessary before starting sawtooth cycle simulations in the presence of fast ions.

HMGC describes the thermal plasma by nonlinear reduced $\mathcal{O}(\varepsilon_0^3)$ visco-resistive MHD equations, with $\varepsilon_0 = a/R_0$ being the inverse aspect ratio (with a and R_0 the minor and major radius of the torus, respectively), evolving the fluctuating electrostatic field ϕ and the perturbed vector potential component, parallel to the equilibrium magnetic field, A_{\parallel} (low- β limit, with β being the ratio of the plasma pressure to the magnetic pressure), in the zero pressure limit. These equations are closed by a pressure term related to one or more particle species (e. g. fast ions), computed by solving the nonlinear gyrokinetic Vlasov equation, in the $k_{\perp}\rho_H \ll 1$ limit (drift-kinetic limit), k_{\perp} being the perpendicular (to the equilibrium magnetic field) wave vector of perturbed fields. HYMAGYC studies energetic-particle driven Alfvénic modes in general high- β axisymmetric equilibria, with perturbed electromagnetic fields (electrostatic potential ϕ and vector potential \mathbf{A}) fully accounted for. The thermal plasma is described by linear, resistive, full MHD equations and the calculations are carried out in flux coordinates (s, χ, φ) , $s = \sqrt{1 - \psi/\psi_a}$ (with $s = 0$ in the center and $s = 1$ at the plasma boundary), ψ is the poloidal flux function, χ is a poloidal angle and φ is the geometrical toroidal angle. The perturbed variables are then expanded using Fourier series in χ and φ , and finite elements in s . When considering two dimensional, axisymmetric equilibria, the solution for each toroidal mode number n is independent from the others, and can be solved one by one. After discretization, one obtains matrices of the coefficients that are block tridiagonal, with eight blocks for each flux-like radial coordinate point considered. The dimension of each elementary block scales with the square of the number of poloidal Fourier components considered (which, in turn, scales as $N_{\text{pol}} \sim n\Delta q$, with $\Delta q = q_{\text{max}} - q_{\text{min}}$, q being the safety factor, and q_{min} , q_{max} the minimum and maximum values of the safety factor considered in the equilibrium, respectively) times the number of equations solved for each flux point. Moreover, also the number of flux points that have to be retained in the simulation, scales with the toroidal mode number n , being the characteristic radial extension of each poloidal Fourier component inversely proportional to n : thus, in turn, the memory requirement to store the matrices of coefficients for solving the linear MHD system scales as n^3 . The MHD field solver originates from the code MARS [76], which has been transformed from an eigenvalue solver to an initial-value one. A parallel version

of this field solver has been implemented in the recent past, thanks to the EFDA-HLST projects PARFS [77, 78] and PARFS2 [79, 80], thus overcoming single-node memory limitations to the maximum toroidal mode number that can be considered in the simulations. The energetic-particle population is described by the nonlinear gyrokinetic Vlasov equation valid for $k_{\perp}\rho_H \sim 1$ (FLR effects properly retained). HYMAGYC is fully interfaced with the European Integrated Modelling Framework [4] data structure and benchmarked against HMGC in the suitable limits [34]. HYMAGYC has also been compared with the hybrid kinetic-MHD MEGA code and fully-gyrokinetic ORB5 code using the NLED-AUG test case to study Alfvénic modes driven by energetic particles [61]. Both HMGC and HYMAGYC are written in Fortran90 and have been parallelized for distributed and shared memory architectures.

For the HYMAGYC code, a strong effort has been put into further IMAS-enabling. In the frame of the European integrated modeling effort [4] and, then, in IMAS [37], a platform for integrated tokamak modeling has been developed using the graphical user friendly Kepler software manager [81]. Within Kepler, interchangeable physics modules, named actors, are used to construct complex Workflows. The minimal HYMAGYCIMAS Kepler Workflow [37] works correctly on the EUROfusion Gateway machine. The UALInit actor is used to extract the required IDS data and pass them to the next HYMAGYCIMAS actor which contains the actual HYMAGYC code. The resulting output of the HYMAGYC simulations is written to the IMAS Database using the UALSliceCollector actor. An extensive optimization of the MHD_LINEAR IDS has been carried out for parallel job executions.

2.3. Integrated modeling

The fully IMASified Energetic-Particle Workflow has been developed and implemented for discharge modelling in ASDEX-Upgrade, JET, and TCV. Predictive studies for JT-60SA and ITER have been performed. The Energetic-Particle Workflow is a pythonic framework coupling transport codes (such as ETS), heating or NBI codes (such as NUBEAM), and self-consistent energetic-particle codes (such as LIGKA/HAGIS) via interfaces based on the IDS data structures. LIGKA [42] is a linear gyrokinetic eigenvalue solver. HAGIS [43] follows the particle guiding-centre orbits providing a self-consistent model for nonlinear wave-particle interaction. The framework has been applied, for example, to the slow LH transition in the ASDEX-Upgrade discharge #39681 in presence of TAE instabilities where both bursty and steady-state phases have been observed. The Energetic-Particle Workflow gains an increasing popularity in EUROfusion's experimental community [82, 83].

As a first step towards a fully integrated simulation of burning plasmas, part of the Energetic-Particle Workflow has been integrated into the transport solver ETS [40] by adding the equilibrium (HELENA) and MHD (LIGKA) Kepler actors in the MHD composite actor. The linear MHD spectrum can now be computed consistently in the convergence loop. To prepare for the integration of more demanding hybrid-kinetic-

MHD or reduced model codes for MHD stability assessment in the presence of energetic particles, the IMASified NBI suite of codes BBNBI/ASCOT/AFSI were revised and upgraded to output in IMAS all the energetic particle distributions relevant for DT burning with sufficient resolution. A first implementation in the kick model limit [44] of the general phase space zonal structure transport equations [84], based on elements of the Energetic-Particle Workflow has been finalised and is currently benchmarked.

In stellarator plasmas, numerical tools for computing ICRH heating and the resulting energetic-particle distribution function have been further developed. The SCENIC code package [47] integrates the ANIMEC [51] (3D MHD equilibrium solver), LEMan [48] (linear full-wave global solver), and the fast-particle code VENUS-LEVIS [49]. Predictive simulations of radio-frequency heating and fast-ion generation have been carried out [85, 47, 86] in Wendelstein 7-X using the SCENIC framework. Finally, a numerical code describing the formation of shear Alfvén continua in stellarator plasmas in presence of magnetic islands has been developed [87]. Continuum calculations play an important role in the reduced modelling of energetic-particle interaction with Alfvénic instabilities and transport.

3. Conclusions

In this paper, we have described the software stack under development within a European coordinated effort on tools for burning plasma modelling. The project is organised as a Task (TSVV Task 10) under the new E-TASC initiative [2]. It is a continued effort within the EUROfusion inheriting from the earlier European coordination projects as well as research projects based at various European laboratories. The ongoing work of the TSVV Tasks is supported by the Advanced Computing Hubs. The major projects requiring the HPC resources are the global gyrokinetic codes ORB5 and EUTERPE. Nonlinear gyrokinetic simulations are performed to address the interaction of fast ions with turbulence and in presence of MHD-like perturbations. Also, we perform linear and nonlinear gyrokinetic simulations to study the mutual influence of MHD/EPM instabilities and energetic ions.

Interaction of energetic particles with the MHD/EPM instabilities can also be addressed using the hybrid particle-MHD codes such as HMGC, HYMAGYC, and XTOR-K. These codes are developed to investigate the role of a large population of fusion alphas and other suprathreshold particles on the global MHD stability limits of the plasma including the impact on the global β -limit of the low- n kink modes stabilization and determination of the sawtooth period in presence of the kinetic effects.

Taking advantage of the IMAS standard, we integrate the hybrid particle-MHD code HYMAGYC into the EUROfusion software eco-system where it can readily be used to analyze "off-line" some temporal snapshots of a transport simulation or even be directly coupled to a transport code, such as the ETS. Such code combination can be used to address self-consistently the mutual interaction of MHD/EPM instabilities driven by fusion alphas and other suprathreshold particles with the respective deposition

profiles and, consequently, with the bulk density and temperature profiles evolution.

On the faster-execution lower-fidelity level, we develop integrated modeling tools which include the IMAS-based Energetic-Particle Workflow (based on HAGIS-LIGKA) and the SCENIC code package computing radio-frequency heating and fast-ion generation. The integrated modelling enables exploration of active strategies to optimize the deposition of alpha particle energy aiming at maximization of the fusion power yield. Furthermore, it enables modelling of burn control through auxiliary heating and fuelling strategies as well as prediction of current profile consistent with bootstrap contributions from pressure profile and fast particles. Reduced models of Alfvénic stability and nonlinear dynamics are being developed for use in the integrated modelling and systems codes addressing Tritium burn-up rates and core plasma Helium content.

In future, we will apply the software stack described in this paper at all fidelity levels to burning plasmas expected in ITER [1], SPARC [88], and also in stellarator-reactor configurations, such as the HELIAS reactor [89], as well as in a DEMO reactor [90]. The software stack developed at the TSVV Task 10 is being made available on EUROfusion's GitLab and on EUROfusion's Gateway which play the role of a central repository and a central "device" for EUROfusion's modeling effort [3]. The training for the Energetic Particle Workflow is planned for EUROfusion's user community.

Acknowledgments

This work has been carried out within the framework of the EUROfusion Consortium, partially funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). The Swiss contribution to this work has been funded by the Swiss State Secretariat for Education, Research and Innovation (SERI). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union, the European Commission or SERI. Neither the European Union nor the European Commission nor SERI can be held responsible for them. This work was supported in part by the Swiss National Science Foundation. We acknowledge PRACE for awarding us access to Marconi100 at CINECA, Italy, and to Joliot-Curie at GENCI@CEA, France. Finally, we thank the organisers of the 3rd Fusion HPC Workshop and, in particular, Edilberto Sanchez, for suggesting this paper.

References

- [1] M. Shimada, D. Campbell, V. Mukhovatov, M. Fujiwara, N. Kirneva, K. Lackner, M. Nagami, V. Pustovitov, N. Uckan, J. Wesley, N. Asakura, A. Costley, A. Donné, E. Doyle, A. Fasoli, C. Gormezano, Y. Gribov, O. Gruber, T. Hender, W. Houlberg, S. Ide, Y. Kamada, A. Leonard, B. Lipschultz, A. Loarte, K. Miyamoto, V. Mukhovatov, T. Osborne, A. Polevoi, and A. Sips, "Progress in the ITER Physics Basis. Chapter 1: Overview and summary," *Nuclear Fusion*, vol. 47, no. 6, p. S1, jun 2007. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/47/6/S01>

- [2] X. Litaudon, F. Jenko, D. Borba, D. V. Borodin, B. J. Braams, S. Brezinsek, I. Calvo, R. Coelho, A. J. H. Donné, O. Embréus, D. Farina, T. Görler, J. P. Graves, R. Hatzky, J. Hillesheim, F. Imbeaux, D. Kalupin, R. Kamendje, H.-T. Kim, H. Meyer, F. Militello, K. Nordlund, C. Roach, F. Robin, M. Romanelli, F. Schluck, E. Serre, E. Sonnendrücker, P. Strand, P. Tamain, D. Tskhakaya, J. L. Velasco, L. Villard, S. Wiesen, H. Wilson, and F. Zonca, “EUROfusion-theory and advanced simulation coordination (E-TASC): programme and the role of high performance computing,” *Plasma Physics and Controlled Fusion*, vol. 64, no. 3, p. 034005, feb 2022. [Online]. Available: <https://dx.doi.org/10.1088/1361-6587/ac44e4>
- [3] P. Strand, R. Coelho, D. Coster, L.-G. Eriksson, F. Imbeaux, and B. Guillerminet, “Simulation and high performance computing — building a predictive capability for fusion,” *Fusion Engineering and Design*, vol. 85, no. 3, pp. 383–387, 2010, proceedings of the 7th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0920379610002310>
- [4] G. Falchetto, D. Coster, R. Coelho, B. Scott, L. Figini, D. Kalupin, E. Nardon, S. Nowak, L. Alves, J. Artaud, V. Basiuk, J. P. Bizarro, C. Boulbe, A. Dinklage, D. Farina, B. Faugeras, J. Ferreira, A. Figueiredo, P. Huynh, F. Imbeaux, I. Ivanova-Stanik, T. Jonsson, H.-J. Klingshirn, C. Konz, A. Kus, N. Marushchenko, G. Pereverzev, M. Owsiak, E. Poli, Y. Peysson, R. Reimer, J. Signoret, O. Sauter, R. Stankiewicz, P. Strand, I. Voitsekhovitch, E. Westerhof, T. Zok, W. Zwingmann, I.-T. Contributors, the ASDEX Upgrade Team, and J.-E. Contributors, “The European Integrated Tokamak Modelling (ITM) effort: achievements and first physics results,” *Nuclear Fusion*, vol. 54, no. 4, p. 043018, mar 2014. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/54/4/043018>
- [5] HLST - High Level Support Team. [Online]. Available: <https://wpcd-workflows.github.io/>
- [6] HLST - High Level Support Team. [Online]. Available: <https://www.efda-hlst.eu/>
- [7] F. Zonca, L. Chen, S. Briguglio, G. Fogaccia, A. V. Milovanov, Z. Qiu, G. Vlad, and X. Wang, “Energetic particles and multi-scale dynamics in fusion plasmas,” *Plasma Physics and Controlled Fusion*, vol. 57, no. 1, p. 014024, nov 2014. [Online]. Available: <https://dx.doi.org/10.1088/0741-3335/57/1/014024>
- [8] L. Chen and F. Zonca, “Physics of Alfvén waves and energetic particles in burning plasmas,” *Rev. Mod. Phys.*, vol. 88, p. 015008, Mar 2016. [Online]. Available: <https://link.aps.org/doi/10.1103/RevModPhys.88.015008>
- [9] L. Chen and F. Zonca, “Nonlinear Excitations of Zonal Structures by Toroidal Alfvén Eigenmodes,” *Phys. Rev. Lett.*, vol. 109, p. 145002, Oct 2012. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.109.145002>
- [10] Y. Todo, H. Berk, and B. Breizman, “Nonlinear magnetohydrodynamic effects on Alfvén eigenmode evolution and zonal flow generation,” *Nuclear Fusion*, vol. 50, no. 8, p. 084016, jul 2010. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/50/8/084016>
- [11] A. D. Siena, T. Görler, E. Poli, A. B. Navarro, A. Biancalani, and F. Jenko, “Electromagnetic turbulence suppression by energetic particle driven modes,” *Nuclear Fusion*, vol. 59, no. 12, p. 124001, sep 2019. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ab4088>
- [12] S. Bernabei, M. G. Bell, R. V. Budny, E. D. Fredrickson, N. N. Gorelenkov, J. C. Hosea, R. Majeski, E. Mazzucato, C. K. Phillips, G. Schilling, and J. R. Wilson, “Nature of Monster Sawteeth and Their Relationship to Alfvén Instabilities in Tokamaks,” *Phys. Rev. Lett.*, vol. 84, pp. 1212–1215, Feb 2000. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.84.1212>
- [13] G. Lo-Cascio, E. Gravier, T. Réveillé, M. Lesur, Y. Sarazin, X. Garbet, L. Vermare, K. Lim, A. Guillevic, and V. Grandgirard, “Transport barrier in 5D gyrokinetic flux-driven simulations,” *Nuclear Fusion*, vol. 62, no. 12, 2022, cited by: 0; All Open Access, Green Open Access. [Online]. Available: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85140293333&doi=10.1088%2f1741-4326%2fac945d&partnerID=40&md5=519ee7385b9d94b46ed2239714aa6644>
- [14] V. Grandgirard, J. Abiteboul, J. Bigot, T. Cartier-Michaud, N. Crouseilles, G. Dif-Pradalier, C. Ehrlacher, D. Esteve, X. Garbet, P. Ghendrih, G. Latu, M. Mehrenberger, C. Nordsieck,

- C. Passeron, F. Rozar, Y. Sarazin, E. Sonnendrücker, A. Strugarek, and D. Zarzoso, "A 5D gyrokinetic full-f global semi-Lagrangian code for flux-driven ion turbulence simulations," *Computer Physics Communications*, vol. 207, pp. 35–68, 2016. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465516301230>
- [15] E. Lanti, N. Ohana, N. Tronko, T. Hayward-Schneider, A. Bottino, B. McMillan, A. Mishchenko, A. Scheinberg, A. Biancalani, P. Angelino, S. Brunner, J. Dominski, P. Donnel, C. Gheller, R. Hatzky, A. Jocksch, S. Jolliet, Z. Lu, J. Martin Collar, I. Novikau, E. Sonnendrücker, T. Vernay, and L. Villard, "ORB5: A global electromagnetic gyrokinetic code using the PIC approach in toroidal geometry," *Computer Physics Communications*, vol. 251, p. 107072, 2020. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0010465519303911>
- [16] N. Ohana, C. Gheller, E. Lanti, A. Jocksch, S. Brunner, and L. Villard, "Gyrokinetic simulations on many- and multi-core architectures with the global electromagnetic Particle-In-Cell Code ORB5," *Computer Physics Communications*, p. 107208, 2020. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465520300461>
- [17] V. Kornilov, R. Kleiber, R. Hatzky, L. Villard, and G. Jost, "Gyrokinetic global three-dimensional simulations of linear ion-temperature-gradient modes in Wendelstein 7-X," *Physics of Plasmas*, vol. 11, no. 6, pp. 3196–3202, 2004. [Online]. Available: <https://doi.org/10.1063/1.1737393>
- [18] A. Biancalani, A. Bottino, P. Lauber, A. Mishchenko, and F. Vannini, "Effect of the electron redistribution on the nonlinear saturation of Alfvén eigenmodes and the excitation of zonal flows," *Journal of Plasma Physics*, vol. 86, no. 3, p. 825860301, 2020.
- [19] A. Biancalani, A. Bottino, A. D. Siena, Ö Gürçan, T. Hayward-Schneider, F. Jenko, P. Lauber, A. Mishchenko, P. Morel, I. Novikau, F. Vannini, L. Villard, and A. Zocco, "Gyrokinetic investigation of Alfvén instabilities in the presence of turbulence," *Plasma Physics and Controlled Fusion*, vol. 63, no. 6, p. 065009, apr 2021. [Online]. Available: <https://dx.doi.org/10.1088/1361-6587/abf256>
- [20] A. Mishchenko, A. Biancalani, A. Bottino, T. Hayward-Schneider, P. Lauber, E. Lanti, L. Villard, R. Kleiber, A. Könies, and M. Borchardt, "Numerics and computation in gyrokinetic simulations of electromagnetic turbulence with global particle-in-cell codes," *Plasma Physics and Controlled Fusion*, vol. 63, no. 8, p. 084007, jun 2021. [Online]. Available: <https://doi.org/10.1088/1361-6587/ac0bcb>
- [21] A. Mishchenko, A. Bottino, T. Hayward-Schneider, E. Poli, X. Wang, R. Kleiber, M. Borchardt, C. Nührenberg, A. Biancalani, A. Könies, E. Lanti, P. Lauber, R. Hatzky, F. Vannini, L. Villard, and F. Widmer, "Gyrokinetic particle-in-cell simulations of electromagnetic turbulence in the presence of fast particles and global modes," *Plasma Physics and Controlled Fusion*, vol. 64, no. 10, p. 104009, sep 2022. [Online]. Available: <https://doi.org/10.1088/1361-6587/ac8dbc>
- [22] F. Vannini, A. Biancalani, A. Bottino, T. Hayward-Schneider, P. Lauber, A. Mishchenko, I. Novikau, and E. Poli, "Gyrokinetic investigation of the damping channels of Alfvén modes in ASDEX Upgrade," *Physics of Plasmas*, vol. 27, no. 4, p. 042501, 2020. [Online]. Available: <https://doi.org/10.1063/1.5134979>
- [23] F. Vannini, A. Biancalani, A. Bottino, T. Hayward-Schneider, P. Lauber, A. Mishchenko, E. Poli, and G. Vlad, "Gyrokinetic investigation of the nonlinear interaction of Alfvén instabilities and energetic particle-driven geodesic acoustic modes," *Physics of Plasmas*, vol. 28, no. 7, p. 072504, 2021. [Online]. Available: <https://doi.org/10.1063/5.0049588>
- [24] F. Vannini, A. Biancalani, A. Bottino, T. Hayward-Schneider, P. Lauber, A. Mishchenko, E. Poli, B. Rettino, G. Vlad, X. Wang, and the ASDEX Upgrade Team, "Gyrokinetic modelling of the Alfvén mode activity in ASDEX Upgrade with an isotropic slowing-down fast-particle distribution," *Nuclear Fusion*, vol. 62, no. 12, p. 126042, nov 2022. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ac8b1e>
- [25] B. Rettino, T. Hayward-Schneider, A. Biancalani, A. Bottino, P. Lauber, I. Chavdarovski, M. Weiland, F. Vannini, and F. Jenko, "Gyrokinetic modeling of anisotropic energetic particle driven instabilities in tokamak plasmas," *Nuclear Fusion*, vol. 62, no. 7, p. 076027, may 2022.

- [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ac6680>
- [26] T. Hayward-Schneider, P. Lauber, A. Bottino, and Z. Lu, "Global linear and nonlinear gyrokinetic modelling of Alfvén eigenmodes in ITER," *Nuclear Fusion*, 2021. [Online]. Available: <http://iopscience.iop.org/article/10.1088/1741-4326/abdca2>
- [27] T. Hayward-Schneider, P. Lauber, A. Bottino, and A. Mishchenko, "Multi-scale analysis of global electromagnetic instabilities in ITER pre-fusion-power operation plasmas," *Nuclear Fusion*, vol. 62, no. 11, p. 112007, sep 2022. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ac6f12>
- [28] M. Sadr, A. Mishchenko, T. Hayward-Schneider, A. Koenies, A. Bottino, A. Biancalani, P. Donnel, E. Lanti, and L. Villard, "Linear and nonlinear excitation of TAE modes by external electromagnetic perturbations using ORB5," *Plasma Physics and Controlled Fusion*, vol. 64, no. 8, p. 085010, jul 2022. [Online]. Available: <https://dx.doi.org/10.1088/1361-6587/ac73eb>
- [29] H. Lütjens and J.-F. Luciani, "XTOR-2F: A fully implicit Newton-Krylov solver applied to nonlinear 3D extended MHD in tokamaks," *Journal of Computational Physics*, vol. 229, no. 21, pp. 8130–8143, 2010. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0021999110003967>
- [30] F. D. Halpern, H. Lütjens, and J.-F. Luciani, "Diamagnetic thresholds for sawtooth cycling in tokamak plasmas," *Physics of Plasmas*, vol. 18, no. 10, p. 102501, 2011. [Online]. Available: <https://doi.org/10.1063/1.3646305>
- [31] G. Brochard, R. Dumont, H. Lütjens, and X. Garbet, "Linear stability of the ITER 15 MA scenario against the alpha fishbone," *Nuclear Fusion*, vol. 60, no. 8, p. 086002, jun 2020. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ab9255>
- [32] V. Kiptily, M. Fitzgerald, Y. Kazakov, J. Ongena, M. Nocente, S. Sharapov, M. Dreval, Z. Stancar, T. Craciunescu, J. Garcia, L. Giacomelli, V. Goloborodko, H. Oliver, H. Weisen, and J. Contributors, "Evidence for Alfvén eigenmodes driven by alpha particles in D-3He fusion experiments on JET," *Nuclear Fusion*, vol. 61, no. 11, p. 114006, oct 2021. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ac26a2>
- [33] F. Zonca, L. Chen, S. Briguglio, G. Fogaccia, G. Vlad, and X. Wang, "Nonlinear dynamics of phase space zonal structures and energetic particle physics in fusion plasmas," *New Journal of Physics*, vol. 17, no. 1, p. 013052, jan 2015. [Online]. Available: <https://dx.doi.org/10.1088/1367-2630/17/1/013052>
- [34] G. Fogaccia, G. Vlad, and S. Briguglio, "Linear benchmarks between the hybrid codes HYMAGYC and HMGC to study energetic particle driven Alfvénic modes," *Nuclear Fusion*, vol. 56, no. 11, p. 112004, jul 2016. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/56/11/112004>
- [35] S. Briguglio, G. Vlad, F. Zonca, and C. Kar, "Hybrid magnetohydrodynamic-gyrokinetic simulation of toroidal Alfvén modes," *Physics of Plasmas*, vol. 2, no. 10, pp. 3711–3723, 1995. [Online]. Available: <https://doi.org/10.1063/1.871071>
- [36] C. Slaby and A. Koenies and R. Kleiber and H. Leyh, "On non-linear frequency chirping in connection with collisions," *Nuclear Fusion*, vol. 59, no. 4, p. 046006, feb 2019. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/aafe31>
- [37] F. Imbeaux, S. Pinches, J. Lister, Y. Buravand, T. Casper, B. Duval, B. Guillerminet, M. Hosokawa, W. Houlberg, P. Huynh, S. Kim, G. Manduchi, M. Owsiak, B. Palak, M. Plociennik, G. Rouault, O. Sauter, and P. Strand, "Design and first applications of the ITER integrated modelling & analysis suite," *Nuclear Fusion*, vol. 55, no. 12, p. 123006, oct 2015. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/55/12/123006>
- [38] H. Lütjens, A. Bondeson, and O. Sauter, "The CHEASE code for toroidal MHD equilibria," *Computer Physics Communications*, vol. 97, no. 3, pp. 219–260, 1996. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S001046559600046X>
- [39] G. Huysmans, J. Goedbloed, and W. Kerner, "Isoparametric Bicubic Hermite Elements for Solution of the Grad-Shafranov Equation," *International Journal of Modern Physics C*, vol. 02, no. 01, pp. 371–376, 1991. [Online]. Available: <https://doi.org/10.1142/S0129183191000512>

- [40] D. Kalupin, I. Ivanova-Stanik, I. Voitsekhovitch, J. Ferreira, D. Coster, L. Alves, T. Aniel, J. Artaud, V. Basiuk, J. P. Bizarro, R. Coelho, A. Czarnecka, P. Huynh, A. Figueiredo, J. Garcia, L. Garzotti, F. Imbeaux, F. Köchl, M. Nave, G. Pereverzev, O. Sauter, B. Scott, R. Stankiewicz, P. Strand, I.-T. contributors, and J.-E. Contributors, "Numerical analysis of JET discharges with the European Transport Simulator," *Nuclear Fusion*, vol. 53, no. 12, p. 123007, nov 2013. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/53/12/123007>
- [41] A. Pankin, D. McCune, R. Andre, G. Bateman, and A. Kritz, "The tokamak Monte Carlo fast ion module NUBEAM in the National Transport Code Collaboration library," *Computer Physics Communications*, vol. 159, no. 3, pp. 157–184, 2004. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465504001109>
- [42] P. Lauber, S. Günter, A. Könies, and S. Pinches, "LIGKA: A linear gyrokinetic code for the description of background kinetic and fast particle effects on the MHD stability in tokamaks," *Journal of Computational Physics*, vol. 226, no. 1, pp. 447–465, 2007. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0021999107001660>
- [43] S. Pinches, L. Appel, J. Candy, S. Sharapov, H. Berk, D. Borba, B. Breizman, T. Hender, K. Hopcraft, G. Huysmans, and W. Kerner, "The hagsis self-consistent nonlinear wave-particle interaction model," *Computer Physics Communications*, vol. 111, no. 1, pp. 133–149, 1998. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465598000344>
- [44] M. Podesta, M. Gorelenkova, and R. B. White, "A reduced fast ion transport model for the tokamak transport code TRANSP," *Plasma Physics and Controlled Fusion*, vol. 56, no. 5, p. 055003, apr 2014. [Online]. Available: <https://dx.doi.org/10.1088/0741-3335/56/5/055003>
- [45] Könies,A. and Slaby,C. and Kleiber,R. and Fehér,T. and Borchardt,M. and Mishchenko,A., "The MHD continuum with a radial electric field," *Physics of Plasmas*, vol. 27, no. 12, p. 122511, 2020. [Online]. Available: <https://doi.org/10.1063/5.0023961>
- [46] S. Hirshman, W. van Rij, and P. Merkel, "Three-dimensional free boundary calculations using a spectral Green's function method," *Computer Physics Communications*, vol. 43, no. 1, pp. 143–155, 1986. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/0010465586900585>
- [47] M. Machielsen, J. P. Graves, and W. A. Cooper, "ICRF modelling in 2D and 3D magnetic configurations using a hot plasma model," *Plasma Physics and Controlled Fusion*, vol. 63, no. 9, p. 094002, sep 2021. [Online]. Available: <https://dx.doi.org/10.1088/1361-6587/ac11b2>
- [48] P. Popovich, W. Cooper, and L. Villard, "A full-wave solver of the Maxwell's equations in 3D cold plasmas," *Computer Physics Communications*, vol. 175, no. 4, pp. 250–263, 2006. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465506001457>
- [49] D. Pfefferlé and W.A. Cooper and J.P. Graves and C. Misev, "VENUS-LEVIS and its spline-Fourier interpolation of 3D toroidal magnetic field representation for guiding-centre and full-orbit simulations of charged energetic particles," *Computer Physics Communications*, vol. 185, no. 12, pp. 3127–3140, 2014. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465514002744>
- [50] L. Eriksson and P. Helander, "Monte Carlo operators for orbit-averaged Fokker-Planck equations," *Physics of Plasmas*, vol. 1, no. 2, pp. 308–314, 1994. [Online]. Available: <https://doi.org/10.1063/1.870832>
- [51] W. Cooper, S. Hirshman, P. Merkel, J. Graves, J. Kisslinger, H. Wobig, Y. Narushima, S. Okamura, and K. Watanabe, "Three-dimensional anisotropic pressure free boundary equilibria," *Computer Physics Communications*, vol. 180, no. 9, pp. 1524–1533, 2009. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0010465509001179>
- [52] A. J. Brizard and T. S. Hahm, "Foundations of nonlinear gyrokinetic theory," *Rev. Mod. Phys.*, vol. 79, pp. 421–468, Apr 2007. [Online]. Available: <https://link.aps.org/doi/10.1103/RevModPhys.79.421>
- [53] J. Horn-Stanja, A. Biancalani, A. Bottino, and A. Mishchenko, "Linear gyrokinetic studies with ORB5 en route to pair plasmas," *Journal of Plasma Physics*, vol. 85, no. 3, p. 905850302, 2019.

- [54] T. Vernay, S. Brunner, L. Villard, B. F. McMillan, S. Jolliet, T. M. Tran, A. Bottino, and J. P. Graves, "Neoclassical equilibria as starting point for global gyrokinetic microturbulence simulations," *Physics of Plasmas*, vol. 17, no. 12, p. 122301, 2010. [Online]. Available: <https://doi.org/10.1063/1.3519513>
- [55] P. Donnel, C. Gheller, S. Brunner, L. Villard, E. Lanti, N. Ohana, and M. Murugappan, "Moment approach of the multi-species non-linear Coulomb collision operator adapted to particle-in-cell codes," *Plasma Physics and Controlled Fusion*, vol. 63, no. 2, p. 025006, dec 2020. [Online]. Available: <https://dx.doi.org/10.1088/1361-6587/abc92b>
- [56] A. Mishchenko, A. Koenies, R. Kleiber, and M. Cole, "Pullback transformation in gyrokinetic electromagnetic simulations," *Physics of Plasmas*, vol. 21, no. 9, p. 092110, 2014. [Online]. Available: <https://doi.org/10.1063/1.4895501>
- [57] R. Kleiber, R. Hatzky, A. Koenies, A. Mishchenko, and E. Sonnendrücker, "An explicit large time step particle-in-cell scheme for nonlinear gyrokinetic simulations in the electromagnetic regime," *Physics of Plasmas*, vol. 23, no. 3, p. 032501, 2016. [Online]. Available: <https://doi.org/10.1063/1.4942788>
- [58] M. D. J. Cole, A. Mishchenko, A. Koenies, R. Hatzky, and R. Kleiber, "A hierarchy of electromagnetic gyrokinetic and fluid hybrid models for the simulation of global modes," *Plasma Physics and Controlled Fusion*, vol. 57, no. 5, p. 054013, apr 2015. [Online]. Available: <https://dx.doi.org/10.1088/0741-3335/57/5/054013>
- [59] N. Tronko, A. Bottino, T. Görler, E. Sonnendrücker, D. Told, and L. Villard, "Verification of Gyrokinetic codes: Theoretical background and applications," *Physics of Plasmas*, vol. 24, no. 5, p. 056115, 2017. [Online]. Available: <https://doi.org/10.1063/1.4982689>
- [60] M. D. J. Cole, A. Biancalani, A. Bottino, R. Kleiber, A. Koenies, and A. Mishchenko, "Toroidal alfvén eigenmodes with nonlinear gyrokinetic and fluid hybrid models," *Physics of Plasmas*, vol. 24, no. 2, p. 022508, 2017. [Online]. Available: <https://doi.org/10.1063/1.4976322>
- [61] G. Vlad, X. Wang, F. Vannini, S. Briguglio, N. Carlevaro, M. V. Falessi, G. Fogaccia, V. Fusco, F. Zonca, A. Biancalani, A. Bottino, T. Hayward-Schneider, and P. Lauber, "A linear benchmark between HYMAGYC, MEGA and ORB5 codes using the NLED-AUG test case to study Alfvénic modes driven by energetic particles," *Nuclear Fusion*, vol. 61, no. 11, p. 116026, oct 2021. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ac2522>
- [62] S. Taimourzadeh, E. Bass, Y. Chen, C. Collins, N. Gorelenkov, A. Koenies, Z. Lu, D. Spong, Y. Todo, M. Austin, J. Bao, A. Biancalani, M. Borchardt, A. Bottino, W. Heidbrink, R. Kleiber, Z. Lin, A. Mishchenko, L. Shi, J. Varela, R. Waltz, G. Yu, W. Zhang, and Y. Zhu, "Verification and validation of integrated simulation of energetic particles in fusion plasmas," *Nuclear Fusion*, vol. 59, no. 6, p. 066006, apr 2019. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ab0c38>
- [63] M. D. J. Cole, A. Mishchenko, A. Bottino, and C. S. Chang, "Tokamak ITG-KBM transition benchmarking with the mixed variables/pullback transformation electromagnetic gyrokinetic scheme," *Physics of Plasmas*, vol. 28, no. 3, p. 034501, 2021. [Online]. Available: <https://doi.org/10.1063/5.0030937>
- [64] X. Sáez, A. Soba, E. Sánchez, R. Kleiber, F. Castejón, and J. Cela, "Improvements of the particle-in-cell code EUTERPE for petascaling machines," *Computer Physics Communications*, vol. 182, no. 9, pp. 2047–2051, 2011, computer Physics Communications Special Edition for Conference on Computational Physics Trondheim, Norway, June 23–26, 2010. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S001046551000531X>
- [65] F. Hindenlang, O. Maj, E. Strumberger, M. Rampp, and E. Sonnendrücker, "GVEC: a newly developed 3D ideal MHD Galerkin variational equilibrium code," *Simons Collaboration on Hidden Symmetries and Fusion Energy*, 2019. [Online]. Available: <https://hiddensymmetries.princeton.edu/meetings/simons-hour-talks>
- [66] E. Sonnendrücker and J. Roche and P. Bertrand and A. Ghizzo, "The Semi-Lagrangian Method for the Numerical Resolution of the Vlasov Equation," *Journal*

- of *Computational Physics*, vol. 149, no. 2, pp. 201–220, 1999. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0021999198961484>
- [67] The PETSc Library. [Online]. Available: <https://petsc.org>
- [68] M. Fitzgerald, S. Sharapov, P. Siren, E. Tholerus, M. Dreval, G. Szepesi, P. Vallejos, T. Johnson, N. Fil, J. Ferreira, P. Rodrigues, A. Figueiredo, D. Borba, R. Coelho, F. Nabais, J. Mailloux, H. Oliver, C. D. Troia, F. Napoli, Z. Stancar, R. Dumont, D. Keeling, and J. Contributors, “Toroidal Alfvén eigenmode stability in JET internal transport barrier afterglow experiments,” *Nuclear Fusion*, vol. 62, no. 10, p. 106001, aug 2022. [Online]. Available: <https://dx.doi.org/10.1088/1741-4326/ac84ee>
- [69] X. Wang, S. Briguglio, C. Di Troia, M. Falessi, G. Fogaccia, V. Fusco, G. Vlad, and F. Zonca, “Analysis of the nonlinear dynamics of a chirping-frequency alfvén mode in a tokamak equilibrium,” *Physics of Plasmas*, vol. 29, no. 3, p. 032512, 2022. [Online]. Available: <https://doi.org/10.1063/5.0080785>
- [70] X. Tao, F. Zonca, and L. Chen, “A “Trap-Release-Amplify” Model of Chorus Waves,” *Journal of Geophysical Research: Space Physics*, vol. 126, no. 9, p. e2021JA029585, 2021, e2021JA029585 2021JA029585. [Online]. Available: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2021JA029585>
- [71] Zonca, F. and Tao, X. and Chen, L., “A theoretical framework of chorus wave excitation,” *Journal of Geophysical Research: Space Physics*, vol. 127, no. 2, p. e2021JA029760, 2022, e2021JA029760 2021JA029760. [Online]. Available: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2021JA029760>
- [72] L. Chen and F. Zonca, “Nonlinear equilibria, stability and generation of zonal structures in toroidal plasmas,” *Nuclear Fusion*, vol. 47, no. 8, p. 886, jul 2007. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/47/8/021>
- [73] A. Bottino, M. Falessi, T. Hayward-Schneider, A. Biancalani, S. Briguglio, R. Hatzky, P. Lauber, A. Mishchenko, E. Poli, B. Rettino, F. Vannini, X. Wang, and F. Zonca, “Time evolution and finite element representation of Phase Space Zonal Structures in ORB5,” *Journal of Physics: Conference Series*, vol. 2397, no. 1, p. 012019, dec 2022. [Online]. Available: <https://dx.doi.org/10.1088/1742-6596/2397/1/012019>
- [74] A. Mishchenko, A. Könies, and R. Hatzky, “Global particle-in-cell simulations of fast-particle effects on shear Alfvén waves,” *Physics of Plasmas*, vol. 16, p. 082105, 2009.
- [75] A. Könies, S. Briguglio, N. Gorelenkov, T. Fehér, M. Isaev, P. Lauber, A. Mishchenko, D. A. Spong, Y. Todo, W. A. Cooper, R. Hatzky, R. Kleiber, M. Borchardt, G. Vlad, A. Biancalani, A. Bottino, and and ITPA EP TG, “Benchmark of gyrokinetic, kinetic MHD and gyrofluid codes for the linear calculation of fast particle driven TAE dynamics,” *Nuclear Fusion*, vol. 58, no. 12, p. 126027, 2018. [Online]. Available: <http://stacks.iop.org/0029-5515/58/i=12/a=126027>
- [76] A. Bondeson, G. Vlad, and H. Lütjens, “Resistive toroidal stability of internal kink modes in circular and shaped tokamaks,” *Physics of Fluids B: Plasma Physics*, vol. 4, no. 7, pp. 1889–1900, 1992. [Online]. Available: <https://doi.org/10.1063/1.860041>
- [77] Abstract of PARFS Project. [Online]. Available: <https://efda-hlst.eu/projects/2012/parfs.html>
- [78] R. Hatzky, “HLST Core Team Report 2012,” EUROFUSION WPISA-REP(16) 16106, Tech. Rep., 2012. [Online]. Available: https://scipub.euro-fusion.org/wp-content/uploads/eurofusion/WPISAREP16_16106_submitted.pdf
- [79] Abstract of PARFS2 Project. [Online]. Available: <https://www.efda-hlst.eu/projects/2014/parfs2.html>
- [80] R. Hatzky, “HLST Core Team Report 2014,” EUROFUSION WPISA-REP(16) 16215, Tech. Rep., 2014. [Online]. Available: https://scipub.euro-fusion.org/wp-content/uploads/eurofusion/WPISAREP16_16215_submitted.pdf
- [81] The Kepler Project. [Online]. Available: <https://kepler-project.org/>
- [82] V.-A. Popa, “Workflow-based energetic particle stability analysis of projected ITER plasmas,” M.Sc. thesis, Technische Universität München, 2021.

- [83] V.-A. Popa, P. Lauber, T. Hayward-Schneider, M. Schneider, O. Hoenen, and S. Pinches, "IMAS - Integrated Workflow for Energetic Particle Stability, submitted," *Nuclear Fusion*, 2023.
- [84] M. V. Falessi and F. Zonca, "Transport theory of phase space zonal structures," *Physics of Plasmas*, vol. 26, no. 2, p. 022305, 2019. [Online]. Available: <https://doi.org/10.1063/1.5063874>
- [85] J. M. Faustin and J. P. Graves and W. A. Cooper and S. Lanthaler and L. Villard and D. Pfefferlé and J. Geiger and Ye. O. Kazakov and D. Van Eester, "Modelling of advanced three-ion ICRF heating and fast ion generation scheme for tokamaks and stellarators," *Plasma Physics and Controlled Fusion*, vol. 59, no. 8, p. 084001, jun 2017. [Online]. Available: <https://dx.doi.org/10.1088/1361-6587/aa72a4>
- [86] C. Slaby, M. Machielsen, S. Lazerson, and J. Graves, "Simulation of radio-frequency heating and fast-ion generation in Wendelstein 7-X," *Journal of Physics: Conference Series*, vol. 2397, no. 1, p. 012006, dec 2022. [Online]. Available: <https://dx.doi.org/10.1088/1742-6596/2397/1/012006>
- [87] A. Könies and J. Cao and R. Kleiber and J. Geiger, "A numerical approach to the calculation of the Alfvén continuum in the presence of magnetic islands," *Physics of Plasmas*, vol. 29, no. 9, p. 092102, 2022. [Online]. Available: <https://doi.org/10.1063/5.0102239>
- [88] A. J. Creely, M. J. Greenwald, S. B. Ballinger, D. Brunner, J. Canik, J. Doody, T. Fülöp, D. T. Garnier, R. Granetz, T. K. Gray, and et al., "Overview of the SPARC tokamak," *Journal of Plasma Physics*, vol. 86, no. 5, p. 865860502, 2020.
- [89] C. Beidler, E. Harmeyer, F. Herrnegger, Y. Igitkhanov, A. Kendl, J. Kisslinger, Y. Kolesnichenko, V. Lutsenko, C. Nührenberg, I. Sidorenko, E. Strumberger, H. Wobig, and Y. Yakovenko, "The Helias reactor HSR4/18," *Nuclear Fusion*, vol. 41, no. 12, p. 1759, dec 2001. [Online]. Available: <https://dx.doi.org/10.1088/0029-5515/41/12/303>
- [90] S.-H. Hong, "A review of DEMO reactor concepts: open questions and issues," *AAPPS Bulletin*, vol. 32, no. 1, p. 10, Apr 2022. [Online]. Available: <https://doi.org/10.1007/s43673-022-00040-9>