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Background

The EU Integrated Modeling (EU-IM) project [1] – and more recently, the ITER Integrated Modelling and Analysis Suite (IMAS) [2,3] – aims to compile a complex simulation program package using standardized interfaces and integration tools to enable the comprehensible simulation of a fusion device and the magnetically confined hot plasma within. IMAS is a worldwide effort aiming to provide a standardized platform and an integrated modelling suite of validated numerical codes for the simulation and prediction of a complete plasma discharge in arbitrary fusion plasma experiments. To address such a challenge, the IMAS approach builds on a modelling infrastructure, focusing on developing a data and communication ontology, i.e. standardizing the data exchange between different codes through a generic data structure incorporating both simulated and experimental data. The main goal of the reported grant was to secure Hungarian participation in the EU-IM and IMAS and consequently to profit from the results of this outstanding effort. The principal investigator and his doctoral students had several years of history in the EU-IM and IMAS projects, both in developing runaway electron modelling actors and in developing the beam emission spectroscopy synthetic diagnostic tools. The principal investigator was also a board member of the EUROfusion Work Package Code Development (WPCD), responsible for running the EU-IM project and its integration into IMAS. Unfortunately, the EUROfusion WPCD was discontinued in 2021, and consequently, the support for its flagship integrated modelling workflow, the European Transport Solver (ETS) [4], became inadequate. This necessitated some changes in the set of tools used for integrated modelling.

One of the main directions of the development concerned runaway electron modelling, which concerned one of the most remarkable characteristics of plasmas. Namely, that the collisional friction force acting on suprathermal electrons decreases with the electron velocity. Therefore, in the presence of a parallel (to the magnetic field) electric field larger than some critical value, electrons with sufficient initial velocity will continually accelerate. The so-called runaway electrons may reach energies in the 10 MeV range [5,6]. As the critical field is proportional to the electron density, runaway electrons are generated in plasma regions of low density and/or large electric field. In particular, they can be produced in great numbers during plasma disruptions, when the rapid cooling associated with a thermal quench gives rise to a large parallel electric field. These runaways are sometimes rapidly lost during the subsequent current quench; in other cases, they form a runaway beam [7]. This beam, which can carry a significant fraction of the initial current, can become unstable and hit the wall over a relatively small area, creating great damage [8]. Understanding the runaway dynamics has been identified as a critical issue for ITER [9]. Even in

present-day tokamaks, the danger of runaway-induced damage often limits the range of operation parameters.

In the simplest runaway models [10], the various processes governing the electron response to a parallel electric field – Spitzer (ohmic) heating [11], Dreicer (primary) runaway generation [5,6], Rosenbluth avalanche (secondary) runaway generation [12], hot-tail formation [13] – are calculated separately, even though these mechanisms are all described by the same electron distribution function and are thus interdependent. In addition, runaway transport due to turbulence [14], resonant magnetic perturbation [15,16,17], kinetic instabilities [18,19], etc, is often calculated based on a given electron distribution without any self-consistent interaction with the runaway generation. An exception is the linearized 3D relativistic finite-difference Fokker-Planck electron guiding-center code LUKE, which was primarily developed to calculate current-drive by RF waves [20,21]. Yet, with non-uniform grids and arbitrary time steps, it is particularly suited to the calculation of runaway dynamics. We planned to continue the collaboration already set up with the developers of the GO [10], LUKE [20,21] and NORSE [22] codes with the aim of code. We aimed to extend the capabilities of a self-consistent simulation of complex plasma systems, the European Transport Simulator (ETS) [23,24], with the modelling of the runaway electron population.

The second planned topic of contribution to EU-IM and IMAS involved the integration of synthetic diagnostic modelling of the atomic beam emission spectroscopy (BES) measurement, which is one of the few tools to measure centimetre scale and microsecond resolved plasma density fluctuations due to plasma turbulence and plasma waves excited by fast particles [25]. The BME group had a long history of simulating BES measurements using the RENATE code [26,27]. A collaboration was also set up with the Denmark University of Technology to apply RENATE as a synthetic diagnostic for the HESEL turbulence code, first outside, then inside IMAS [28]. This plasma turbulence with synthetic diagnostic workflow was planned to be generalized to more turbulence and non-linear MHD codes with the primary goal of aiding their validation. Validation efforts were to be aided by another traditional field of activity of the BME group: the characterization of plasma transients by advanced signal processing methods based on continuous linear time-frequency transforms, like short-time Fourier and analytical wavelet transform [29,30], also utilized for the experimental validation of theoretical models [31,32].

Research practices

For programming, we mostly use the online infrastructure provided for open-source code development. For runaway codes: <https://github.com/osrep>, <https://github.com/hoppe93/NORSE>, <https://github.com/chalmersplasmatheory/DREAM>, <https://github.com/hoppe93/SOFT>, while for the BES synthetic diagnostic <https://github.com/gergopokol/renate-od> and <https://github.com/cherab>. The repository management and issue tracking system provided by GitHub is supplemented by the Travis continuous integration tool. For specific interfacing to IMAS modules, we used the infrastructure provided by ITER and EU-IM. The proposed tasks relied heavily on the infrastructure and the integrated modelling framework provided by EUROfusion WPCD, whereas after its cancellation, the ITER Organization and the Chalmers University of Technology were approached as a backup solution. The resources of ITER and Chalmers were successfully combined, which opened the way to new EUROfusion involvements.

Research results

Our effort into the integration of runaway electron models into the EU-IM and IMAS integrated modelling frameworks started by porting the codes into the respective high-performance computing environments and then writing a wrapper to interface them to the standardized data structures. The integration was then tested in test workflows, used in verified in specialized workflows, and finally integrated into the integrated modelling workflows – later being ETS5 on the EU-IM infrastructure of ETS6 on IMAS.

The codes themselves were either self-developed, like Runaway Indicator and Runaway Fluid [4,33], or developed by our collaborators, like NORSE [22] or DREAM [34]. Research methods for modelling runaway electrons were based on either analytical work or numerical studies on the Fokker-Planck equation for runaway electrons. Runaway Indicator and Runaway Fluid used a fluid-like description resulting from analytical solutions of the runaway electron generation rates. This description is similar to the one used in the GO code, which was the first self-consistent disruption simulator developed at Chalmers [10]. NORSE, on the other hand, used a numerical solver for the non-linear Fokker-Planck equation [22], while DREAM could calculate either with fluid-like description or a linearized Fokker-Planck numerical solver [34]. The applicability of this range of models has been explored in detail in a paper by my doctoral student, Soma Olasz [35]. An important conclusion was that the frequently applied fluid-like models are correct only for cases when the time scale of the plasma parameter changes is longer than the electron slowing down collision time at the critical velocity for runaway formation. This condition is often violated in the thermal quench phases of tokamak disruptions.

Having the integration of Runaway Indicator, Runaway Fluid and NORSE into IMAS completed, it became possible to include those into more comprehensive transport workflows capable of self-consistent modelling of plasmas. Such a 1.5D transport simulator was the European Transport Simulator (ETS) [23, 24]. Preliminary results have shown good agreement with expectations, but the adoption of the workflow to disruption scenarios would have needed improvements in numerical stability [35]. This effort stopped when EUROfusion stopped financing the development of ETS, and we had to move on to a different self-consistent disruption simulator. Our choice was DREAM, which has just been developed into a self-consistent solver by adding atomic physics and transport models [34]. After some preliminary studies, we began running DREAM with the kinetic model for runaway electrons. This has not only provided the runaway current as output but also the 2D bounce-averaged distribution function. Having the distribution function enabled us to produce synthetic camera images resulting from the synchrotron radiation of the runaway electron beam using the SOFT synthetic diagnostic [36]. We first took part in a study using SOFT done for ASDEX-Upgrade [37] and then used the combination of DREAM and SOFT for predictive simulations of the EDICAM camera system at the JT-60SA tokamak [28, 39, 40]. We have predicted that it would be possible to detect a runaway electron beam, which was later also indicated in the commissioning campaign of JT-60SA, but the measurement results are still under embargo.

Development of the beam emission spectroscopy (BES) synthetic diagnostic was very much facilitated by having our own validated beam emission simulator, RENATE [25-27]. Both RENATE and its successor, RENATE-OD, have benefited from improved atomic physics cross-sections and benchmarks in the IAEA CRP F43023 on Data for Atomic Processes of Neutral Beams in Fusion Plasma (2016-2020) collaboration, which actually ended in 2023 with a summary paper [41]. In the

course of the project, we took part in the calculation and validation of improved cross-sections [42], but our main effort was focused on benchmarking the different beam emission and beam attenuation codes. The main conclusions were that all of the studied codes are in agreement regarding the modelling of the attenuation of hydrogen atomic beams in fusion-grade plasmas within the uncertainty of the atomic data. However, there are significant differences in handling impurities, which might require further improvements in the future [40,43,44].

Our improved simulation capabilities were utilized in a large number of studies aiming for a better understanding of existing BES systems and for feasibility studies of proposed BES systems around the world. A summary of these is given in the doctoral thesis of one of the doctoral students of the principal investigator, Örs Asztalos [45]. The most recent application for existing diagnostics is for the Wendelstein 7-X stellarator [46,47], while feasibility studies have been performed for the JT-60SA tokamak [48] and the HSX stellarator [49].

The work done for the HSX stellarator [49] has initiated a study on the behaviour of alkali beam emission spectroscopy in low-ion-temperature plasma. In such plasmas, there is a strong temperature dependence of the slower beam atoms (e.g. in sodium beams of low energy lithium beams), which makes the evaluation of BES measurements more challenging, but could also enable the measurement of temperature, whereas only the density can be measured by BES in normal conditions. This might open possibilities in the diagnostics of tokamak divertor regions in the future [50].

The extension of our cross-section database to include neutral-neutral collisions [41] has enabled us to investigate the feasibility of measuring the neutral content of the edge plasma of tokamaks and stellarators. The calculations have shown that this would be possible if we had the right optical system and a high neutral fraction due to either gas puff fueling or other transient events [51]. We expect to have proof-of-principle experiments this year.

RENATE was used not only in the simulation of BES measurements but also in the simulation of slightly different diagnostic systems. One such sister diagnostics is the atomic beam probe (ABP), which relies on detecting the large Larmor-radius alkali ions, whose source is the injected alkali atomic beam. Due to their large Larmor radius, these ions exit the plasma and can be detected by Faraday-cup-like detectors placed near the plasma edge. The trajectory of the ions is affected by the magnetic field fluctuations along its path, so this arrangement could be used to detect current filaments in the future. RENATE was used in the related numerical studies to calculate the place of ionization, which is the start of the ion orbits [52].

Our BES modelling capabilities are now being developed in two directions. One direction is the inclusion of machine learning methods into the solution of the rate-equations. There were good results with neural-network-like models in the prediction of light emission from alkali beams penetrating the edge plasma [53]. In the short run, the application of machine learning is expected to speed up our BES synthetic diagnostic by orders of magnitude, thus making it more suitable for the task of validating first-principle plasma simulations. In the long run, the direction of modelling might be reversed, and machine learning could be used in the evaluation of the BES measurements. We have just submitted a proposal on the subject to EUROfusion.

The other direction of development is the spectral modelling of the BES spectrum. This is made challenging by the perceived electric field of the high-velocity beam atoms, causing a Stark splitting of the emission lines. This motional Stark effect (MSE) is used in dedicated MSE diagnostics to measure the magnetic field along the atomic beam path. A simulation tool capable of simulating the MSE spectra has been developed by Péter Balázs, a doctoral student of the principal investigator, in collaboration with ITER [54]. Benchmarking with other simulation tools and an application to refine our BES feasibility study for ITER is ongoing [55].

One of the aims of the BES synthetic diagnostic development was to employ it to validate first-principle plasma turbulence and non-linear MHD codes. A “Turbulence plus synthetic diagnostics” workflow has been developed for this purpose and used for validating the HESEL scrape-off-layer turbulence code [56]. Work is ongoing to continue the effort of validation of HESEL [28] and use its predicted fluctuating plasma parameter distributions for feasibility studies of future BES systems in ITER and JT-60SA [48]. First, studies of using the BES synthetic diagnostics on outputs non-linear MHD codes have been demonstrated on JOEKE simulations for JT-60SA [48], but a collaboration has been set up to conclude actual validation studies on MAST Upgrade. The development of the aforementioned machine learning capabilities [53] will be invaluable for this undertaking.

Conclusion

The project has supported the employment of the principal investigator and research projects of 3 doctoral students and 4 undergraduate students. The results were summarized in 8 journal papers and 14 conference contributions. The research goals of the first two years were completed as planned, and then an adjustment of the goals was needed because of the phasing out of the EU-IM integrated modelling infrastructure. Significant new results have been achieved in both the runaway electron modelling and the beam emission synthetic diagnostic areas, which has formed a good basis for further international collaborations. This manifested in the official involvement in the EUROfusion work package for DEMO design with the task of runaway electron modelling, a EUROfusion Researcher Grant position awarded to Örs Asztalos in the area of synthetic diagnostic development, an Implementing Agreement with the ITER Organization on diagnostic modelling and design, and two ITER Internships for the involved students.

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