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An overview of the evolution of the modeling of reflectometry diagnostics in fusion plasmas using finite-difference time-domain codes

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ABSTRACT

Microwave reflectometry, having its origins in ionosphere probing techniques to evaluate electronic density, has become one of the most important diagnostics for the same quantity in fusion plasmas. Reflectometry will play a major role in next-generation machines, in particular in DEMO, where it is expected to provide plasma positioning, shaping, and tracking data. The ability to have an ever-increasing comprehensive description of reflectometry is particularly important since it allows us to assess the measuring capabilities of existing experimental systems and to predict the performance of new diagnostic concepts based on probing waves. Furthermore, wave propagation in a thermonuclear plasma with fluctuating electronic densities is far from straightforward and the need for a numerical full-wave treatment becomes fundamental. We will present the reader with the fundamentals of this technique and introduce the usage and evolution of FDTD in reflectometry, using as an example, the synthetic diagnostics setup that uses the family of REFMUL* codes, which is employed in the assessment of the performance of several reflectometry systems in different fusion machines.

1. Introduction and objectives

Microwave reflectometry, having its origins in ionosphere probing techniques [1], has become one of the most important tools in fusion plasmas to diagnose the electronic density n_e [2,3]. This diagnostic will play a major role in next-generation machines, in particular in DEMO, where it is expected to provide plasma positioning, shaping and tracking data [4]. This goal implies going through an intensive research process to answer many still-open questions and to tackle new ones that no doubt will appear in fusion reactor applications. Simulation codes and synthetic diagnostics play already an extremely important role that will increase in the future. The ability to have an ever-increasing comprehensive description of reflectometry is particularly important since it allows to assess the measuring capabilities of existing experimental systems and to predict the performance of future ones. A thermonuclear plasma is a *unforgiving* difficult media, making the description of wave propagation in it a monumental task, as will be developed further down the text. As if such was not enough, as simulations of full systems advance, the influence of the *hardware* (antennas, waveguides, access to vacuum vessel, first wall) becomes evident, with the likely appearance of resonances, multi reflections, and multimode generation, whose impact on the signals must be accounted. Analytical descriptions have clear limits and simply cannot cope with such rich and complex phenomena. A full-wave treatment is fundamental. Different Computational ElectroMagnetic (CEM) techniques have been used to address these demands, being finite-difference time-domain (FDTD) using Yee's scheme one of the most efficient. Different kinds of full-wave codes are compared in [5]. In the remainder of the paper we will introduce the reader to the fundamentals of reflectometry and to the usage and evolution of FDTD in reflectometry, using as an example, the setup of a synthetic diagnostic with the family of REFMUL* codes, employed in the assessment of the performance of several reflectometry systems in different fusion machines.

2. Reflectometry

Microwave reflectometry depends on the propagation of an electromagnetic wave in a plasma. Several different techniques are used in reflectometry, such as fixed frequency, Doppler reflectometry, hopping

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reflectometry, pulse reflectometry, amplitude-modulated reflectometry or frequency-modulated continuous-wave reflectometry (FMCW) [2,6,7]. We will briefly describe the principle of reflectometry referring to this last technique, FMCW, since it is presently the main one being used for density profile evaluation, needed for Plasma Position Reflectometry (PPR), and foreseen for next-generation machines [8]. It involves the launching, perpendicularly to the separatrix, of a probing signal, $S_{tx} = A_{tx}\cos(\omega t)$, into the plasma, where it propagates prior to being reflected at a cutoff layer and returning to the emitting antenna (monostatic setup) or to a separate receiving antenna placed beside the former (bistatic setup). The received signal, $S_{rx} = A_{rx}\cos(\omega t + \varphi)$, differs from the emitted one in amplitude and in phase. The phase difference, $\varphi = \varphi_\mu + \varphi_0 + \varphi_p$ encompasses the signature of the microwave circuit, φ_μ, which is known through calibration, the contribution of the propagation in vacuum, φ_0 a value that can be evaluated and the signature of the propagation in the plasma, φ_p which conveys the main information we are looking for. φ_p captures the propagation along a path described by a refractive index $N(\mathbf{r})$ and contains information on the electronic density n_e. The Altar-Appleton equation (aka Appleton-Hartree or Appleton-Lassen) describes the refractive index of a wave propagation in a cold magnetized plasma [9], where a magnetic field $\mathbf{B_0}$ exists. Of interest to reflectometry is the particular case of propagation perpendicular to the external magnetic field $\mathbf{k} \perp \mathbf{B_0}$, which gives two expressions. One for the ordinary mode (O-mode) with $N_O^2 = 1 - X$ and another for the extraordinary mode (E- or X-mode) with $N_X^2 = 1 - X(1 - X)/(1 - X - Y^2)$ [10]. Note the normalization $X = \omega_p^2/\omega^2$ and $Y = \omega_c/\omega$, where ω_p, ω_c and ω are the plasma, the electron cyclotron and the wave angular frequencies, respectively. In the WKBJ framework ignoring the scattering effects, the O-mode describes a linear polarized wave with its electric field parallel to $\mathbf{B_0}$ $(\mathbf{E}//\mathbf{B_0})$ while the X-mode describes an elliptical polarization with the wave electric field perpendicular to $\mathbf{B_0}$ $(\mathbf{E} \perp \mathbf{B_0})$. For the O-mode, the phase due to the plasma propagation, φ_p, is a function of the wave frequency f and the plasma electronic frequency ω_p, $\varphi_p[f, N_O(n_e)]$, while for the X-mode also depends on $\mathbf{B_0}$, $\varphi_p[f, N_X(n_e, B_0)]$ [7,11].

3. Why are complicated simulation codes necessary?

According to the previous introduction, it would appear that the accurate mathematical description of wave propagation in plasmas offers the necessary tools for interpreting reflectometry. If that is the case, why is so much effort spent on creating sophisticated simulation codes? It turns out that the analytic solutions describing propagation in plasmas depend on simplifying assumptions and the resulting *ideal* situation on the basis of mathematical descriptions exists, in fact, only in textbooks like [10]. In reality, wave propagation in a thermonuclear plasma is far from trivial. Such a plasma is typically an inhomogeneous, non-stationary, and anisotropic environment exhibiting an exceedingly complex behavior, wherein the propagating wave is subject to the effects of turbulence, magnetohydrodynamics, Doppler shifts, absorption, diffusion, and mode conversion, just to mention a few. Even a simple $2D$ simulation can reveal a multitude of phenomena, impossible to assess analytically, such as multi-scattering; appearance of local resonances; secondary cutoffs; beam splitting; and wave trapping that can destroy the coherence of the probing beam. Another reason to use codes is to assess the complex interaction between the plasma and the ensemble of the antennas, first wall, and access to the vacuum vessel. Even assuming an *idealized textbook* quiescent plasma, complicated resonances and multi-reflections can arise within the access apertures, antennas, and oversized waveguides, or between the wall and the plasma. An accurate representation of the hardware and its effects is thus of paramount importance. Only a 3D full-wave inclusion of the reflectometer moke-up structure is able to recover the amplitude and phase measurements, as it takes into account the anisotropy of the radiation pattern, not present in a 2D code. This is well illustrated by DTT reflectometer moke-up [12]. Usually, the main quantity looked for is phase. Nevertheless, in some situations, amplitude can be a crucial part of the measurement and only 3D full-wave can provide a representative synthetic diagnostic, as in the case of MILS, for instance, [13].

FDTD has become, in the past thirty years, one of the major numerical methods to solve problems of electromagnetism in general, including in the area of wave propagation. As floating point operation (FLOP) costs decrease, new applications of FDTD appear, making it an important research area, with constant extensions and improvements to the base techniques being developed. For the applications we are interested in, namely propagation of an electromagnetic wave in a plasma [14] and, more specifically, on reflectometry, the use of FDTD codes has also found its place [15] and is being employed with success in an increasing number of problems. The term FDTD when used in the context of wave propagation usually refers to the numerical resolution of Maxwell curl equations (Ampere's and Faraday's laws) (FDTD-Maxwell). The solving of a wave equation can also be done using FDTD (FDTD-Wave-Equation) [16].

4. The REFMUL* code family

REFMUL* is a package of FDTD Maxwell full-wave codes, that started being developed around 2000. The first code was REFMUL, a 2D O-mode simulation code [17], followed some years later by REFMULX/REFMULXp: 2D X-mode (serial/parallel) simulation codes [18]. Both codes are in a phase-out stage and are being replaced by REFMULF, a 2D code, and REFMUL3 a 3D code.

4.1. REFMULF, a 2D full-wave code

REFMULF, like the *traditional* 2D O- and X-mode codes, also considers propagation in a 2D plane (x-y plane) with no gradients along z $(\partial/\partial z = 0)$. Maxwell equations are solved using the classic Yee schema [19] but using instead two simultaneous sets of staggered grids, one for the transverse magnetic mode (TMz) with field components E_z, H_x and H_y, and another for the transverse electric mode (TEz), with field components H_z, E_x and E_y. REFMULF is able to cope with full polarization waves, treating all components of $\mathbf{E}(x, y) = E_x\mathbf{e_x} + E_y\mathbf{e_y} + E_z\mathbf{e_z}$ and $\mathbf{H}(x, y) = H_x\mathbf{e_x} + H_y\mathbf{e_y} + H_z\mathbf{e_z}$ of the wave. It supports a generic external magnetic field $\mathbf{B_0}(x, y) = B_{0_x}\mathbf{e_x} + B_{0_y}\mathbf{e_y} + B_{0_z}\mathbf{e_z}$, coupling the Transverse-Electric Mode (TE, X-mode) with the Transverse-Magnetic Mode (TM, O-mode) via a linear vector differential equation for $\mathbf{J}(x, y)$, which is solved using a modified Xu-Yuan kernel [20,21]. The modification of the Xu-Yuan kernel allows extended long-run stability, despite introducing numerical advection effects. The components of the external magnetic field $\mathbf{B_0}$ lying on the propagation plane are responsible for linking the TE and TM modes and thus are able to describe oblique propagation. The major difference from *classic* 2D codes is that a generic external magnetic field $\mathbf{B_0}(xy) = B_{0_x}\mathbf{e_x} + B_{0_y}\mathbf{e_y} + B_{0_z}\mathbf{e_z}$ is now allowed. This permits coupling of the TMz and TEz planes via the external product $\boldsymbol{\omega}_c \times \mathbf{J}$ occurring in the linear differential equation for the current density, since $\mathbf{J}(x, y) = J_x\mathbf{e_x} + J_y\mathbf{e_y} + J_z\mathbf{e_z}$ and $\boldsymbol{\omega}_c(xy) = \omega_x\mathbf{e_x} + \omega_y\mathbf{e_y} + \omega_z\mathbf{e_z}$, considering that $\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}$. Note that the direct coupling through Maxwell equations is not possible because $\partial/\partial z = 0$. This *indirect* coupling enlarges the possibilities of simulation of microwave reflectometry offering capabilities unavailable in present-day 2D reflectometry codes, such as coupling O/X, useful to describe the effect of magnetic fluctuations [22] or to describe OXB heating scheme [23], Faraday rotation [7,10] and Cotton-Moutton effect [7], for instance. Otherwise, for a $\mathbf{B_0}$ purely perpendicular to the propagation plane, the code describes simultaneously two separated planes of O-mode and X-mode propagation. If only one of the modes is to be simulated, the code can be compiled as a *traditional* O- or X-mode code, using only the corresponding plane and the appropriate set of reduced equations, allowing for a faster runtime and a lower memory footprint. REFMULF has different types of sources, on both planes: Unidirectional Transparent Source (UTS) [17], used in the implementation of antennas/waveguides emitting structures [17], Total Field-Scattered Field (TFSF) plane wave, and Periodic Boundary Condition (PBC) plane wave.

REFMULF is not far from a full polarization 3D code. In fact, if we overlay N TEz planes intermediated by $N-1$ TMz planes, instate dependency on z, e.g., $\mathbf{J} = \mathbf{J}(x, y, z)$, and allow for variation along the z axis ($\partial/\partial z \neq 0$) we obtain the basis of REFMUL3.

4.2. REFMUL3, a 3D parallel code

REFMUL3 includes all of the wave field components and a generic external magnetic field. It has a 3D domain decomposition for a parallel hybrid implementation, using Message Passing Interface (MPI) together with Open Multi-Processing (OpenMP). Recently, it has been extended to run on GPUs using OpenMP offloading. The code's output is parallel, written in either the Hierarchical Data Format (HDF5) with an eXtensible Data Model Format (XDMF) wrapper for the data description, or alternatively, in the Visualization Toolkit (VTK) format including compression. REFMUL3 exhibits a very good performance and scales rather well as can be observed from Fig. 1, where the strong scaling (keeping the simulation size constant and increasing the number of resources used in parallel) curves are shown for a 2000 × 1500 × 1500 simulation on CINECA'S Marconi (Skylake partition) High Performance Computer (HPC). Note that this is a case involving a grid of 4500 million points. On the bottom of Fig. 1, the performance results for a 5867 × 1067 × 1067 grid size are shown, corresponding to a volume of 6,679,514,963 million points. The wallclock run times on Marconi Skylake are represented by the orange bars while the green bars refer to the runtime on the new CINECA's the pre-exascale Tier-0 EuroHPC supercomputer Leonardo. The benefit of the recent extension of REFMUL3 to enable using GPUs is clear.

Along with the progress of the codes and kernels, the need to faithfully represent the *hardware* part of the full system becomes more and more evident. These synthetic diagnostics need realistic representations of all system components to incorporate the main effects that shape their behavior. Some of the most important elements that are required to be well modeled and integrated in simulations are the wave launcher structures, such as the waveguides, tapers, and antennas, as well as the vessel wall structures and access to the plasma. The latter are of paramount importance and are often neglected in this type of study. Faithfully modeling them is not an easy task, especially in 3D simulations. A 3D CAD model input pipeline for REFMUL3 has been developed to convert complex CAD models of tokamak vessel components and wave launcher structures to the VOXEL input required by REFMUL3 [12].

Not only closely associated with, but rather what in fact allows the evolution of code dimensionality, is the progress in computer power and the computational resources availability. One-dimensional codes can run comfortably on a 1980's portable computer. Two-dimensional codes raise the bar a notch and will need a modern workstation. For three-dimensional synthetic reflectometry, one needs access to high-performance computers, such as the aforementioned CINECA's Marconi or Leonardo. The reason lies in the small spatial discretization of large volumes with the associated small temporal discretization.

5. Illustration of the requirements and constraints for REFMUL3

To work out an example, let us consider a physical volume of $0.76\,\mathrm{m} \times 0.51\,\mathrm{m} \times 0.51\,\mathrm{m}$, sampled with 40 points/wavelength, $\delta_{x,y,z} = 40/\lambda_0$. If we consider a $2D$ x-y plane cut, for the K band $\delta_{x,y,z} = 5.66 \times 10^{-4}\,\mathrm{m}$, which gives a grid size of 1348×899 (1,211,852 grid points), a fairly trivial problem nowadays. For the W band, the highest band we use, $\delta_{x,y,z} = 1.36 \times 10^{-4}\,\mathrm{m}$ yields a grid size of 5588×3750 (20,955,000 grid points), more demanding but still manageable. Once we pass to $3D$, the K band implies a grid size volume of 1348 × 899 × 899 (1,089,454,948 grid points), while for the W band, the grid would be 5588 × 3750 × 3750 (78,581,250,000 grid points). These physical area/volume values are the ones involved in the 2D and 3D simulations for assessing a Low Field Side (LFS) PPR for Divertor Tokamak Test facility (DTT) [24,25] shown in Fig. 2. The 3D simulations ran on Marconi Skylake partition on 64 nodes (3072 cores) with 4 MPI tasks per node (256 MPI tasks in total) and 12 OpenMP threads per task. The K band took 7 h, while the Ka band needed around 40 h, run in two consecutive job submissions of 20 h each. The 3D simulations were done just for the K and Ka bands, not because the simulation of the higher bands was not feasible but for a more mundane reason, the exhaustion of the budget of CPU hours available for the project at that HPC facility. The 2D simulation was done on a single Marconi Skylake node, using 48 OpenMP threads, taking about 7 min for the K band and up to 1 h:30 m for the W band.

6. Discussion

We are presently living in very auspicious times, in which Nuclear Fusion is under the spotlight with the recent fusion power record achieved at the Joint European Torus (JET) located at the Culham Centre for Fusion Energy [26] and with the achievement of fusion ignition at the National Ignition Facility (NIF) located at the Lawrence Livermore National Laboratory [27]. ITER construction advances fast with the start of the assembly of the vacuum vessel. Plans for next-generation machines are afoot. The need to prepare reflectometry systems for these coming machines, where they are foreseen to play a major role, is driving an effort to have better and better synthetic diagnostics. In addition to better 2D codes, able to include more aspects of fundamental physics, such as REFMULF, there is a clear perception that a full understanding of a real system needs a 3D description. With REFMUL3, this transition from 2D to 3D is being done and this code is of great interest to the reflectometry community, as an essential tool to capture the full description of a reflectometry diagnostic. It is particularly suitable for studies on the amplitude of reflected signals because the true geometry of the probing beam is taken into account. It can also account for possible resonance contributions due to the surrounding geometry, which are important in the case of plasma position reflectometers inserted in the machine blanket. The latest simulations using REFMUL3 [28] present an integrated design workflow for a PPR diagnostic system, using CAD models of antennas and first-wall components, incorporates 3D advanced full-wave simulations in target plasma scenarios, and includes laboratory tests of laser metal printed antennas prototypes. Comparison of simulation of the antennas with laboratory tests of 3D printed mockups attest to the very high degree of realism and absolute accuracy achievable with the synthetic diagnostic based on the REFMUL3 simulator. REFMUL3 has recently been used by a third party as one of the codes to benchmark and validate the Leonardo HPC system [29]. Since the need and will to simulate real machine systems appeared, it became clear that only a good description of the antenna behavior could lead to relevant results, first felt in 2D [30–32] and confirmed with these latest 3D results [25,28]. It is high time to stop using synthetic beams or screen sources to implement a synthetic diagnostic. These techniques have undoubtedly their areas of validity and application, nevertheless, synthetic reflectometry is not one of those. A description of the full system requires also a consistent model for the plasma and a fair amount of time has been devoted to the inclusion of the plasma description in the simulation. Firstly with built-in plasma models accounting for different plasma profiles, density perturbations, or turbulence. More recently, the latest works devoted to PPR simulation in different machines include realist scenarios given by equilibria codes that must be adapted to be used as inputs to REFMUL*'s codes [24,32]. A parallel effort includes the results given by sophisticated codes describing the plasma behavior, such as GEMR [33,34], a gyrofluid code computing the evolution of density turbulent fluctuations and the density profile gradient [35], or JOREK [36], a non-linear MHD code [37] as inputs to REFMUL* codes.

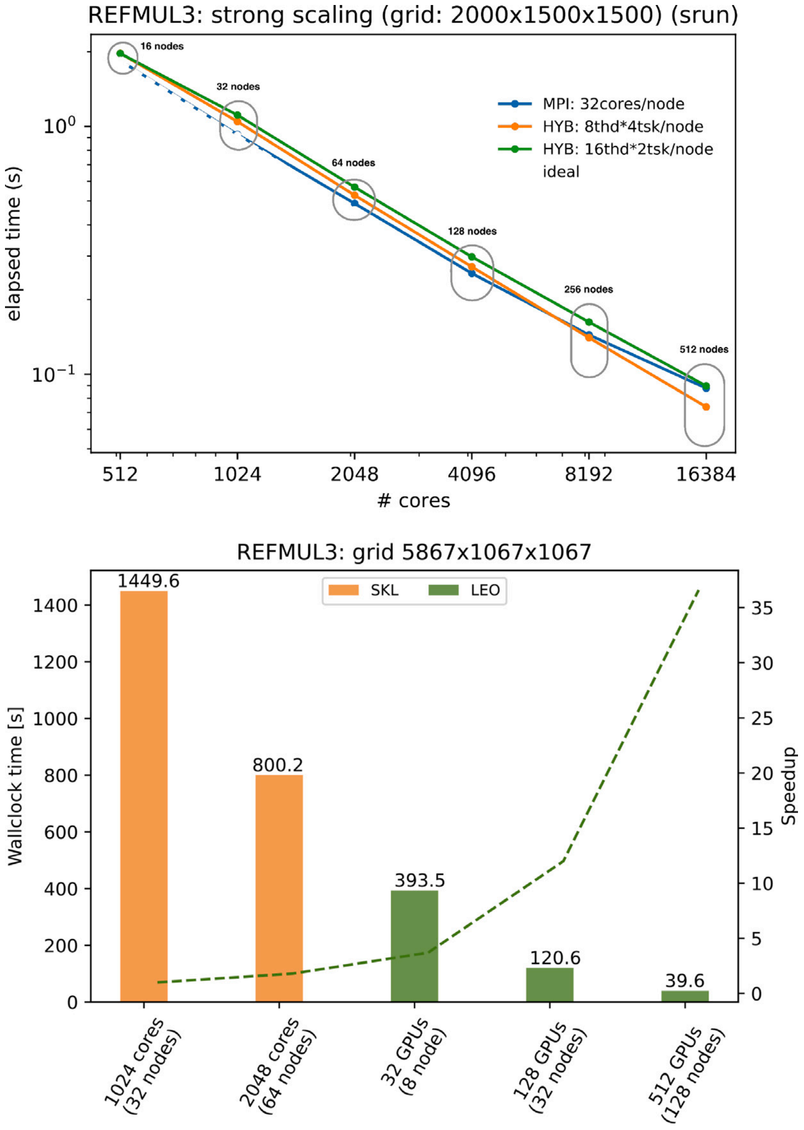

Fig. 1. On the top, the strong scaling behavior on Marconi's Skylake (SKL) partition for different combinations of MPI tasks and OpenMP threads. The bottom graphic displays a comparison of wallclock times on CINECA's SKL in orange and on Leonardo (LEO) in green. The green dashed line shows the speedup factor (y-axis on the right) with respect to the simulation on 32 Skylake nodes (leftmost orange bar).

Around the 2000's, an effort was undertaken to pass from 1D simulations to 2D, bringing synthetic diagnostics along the poloidal plane, incorporating 2D effects, and allowing the use of more detailed 2D structures and antenna designs. A similar path is being presently attempted to achieve 3D simulations to provide a realistic volumetric simulation that incorporates the full 3D effects affecting the waves propagating in the plasma, and their interaction with the more or less complex geometries of the launcher and receiver antennas, vessel wall antenna access cutouts, and other surrounding plasma facing structures. A major difference is that while the former transition to 2D could be made locally at the office, in the lab, or at home, with a good desktop, the present evolution to 3D is more complex, since the developer needs, not only the knowledge concerning computational physics, but also the capacity to produce highly optimized parallel codes able to run efficiently on modern HPC facilities. Another related point refers to the sheer amount of output data that is typically produced during a large 3D simulation, which requires a highly optimized parallel implementation to avoid becoming a bottleneck during runtime. The user of such codes needs also the extra expertise to use such an HPC machine, namely on how to log and understand the work environment, modules system, compilation, and job schedulers, as well as modern visualization tools, for instance. Another important point to have in mind is that in large projects, involving launching a massive number of simulations, whose inputs must be prepared and the results analyzed, there is a need to automatize all these processes and to keep a methodic bookkeeping [38]. Equally important is how to gain access to an HPC facility, an additional burden. It may involve buying simulation hours, being involved in a project with access to an HPC, or answering a call for HPC use, for instance, EUROfusion HPC, PRACE, or JU-EUROPC. In any case, the user should be prepared for some paperwork involved in answering technical and bureaucratic demands and subsequently writing reports, not to mention accommodating the possibility of being granted fewer resources than initially anticipated. Research of new numerical kernels is also an area where important developments keep appearing with the adaptation of proven kernels to reflectometry [20] or the writing of new ones [21].

It is now more than evident that next-generation HPC machines will rely heavily on the use of GPUs and FDTD is a numerical technique appropriate to the massively parallel computations they provide. There is a need to write new codes or to efficiently adapt or rewrite existing ones to take advantage of this new paradigm. Good examples of such are REFMUL3, as shown above, or CUWA, a FDTD code developed to

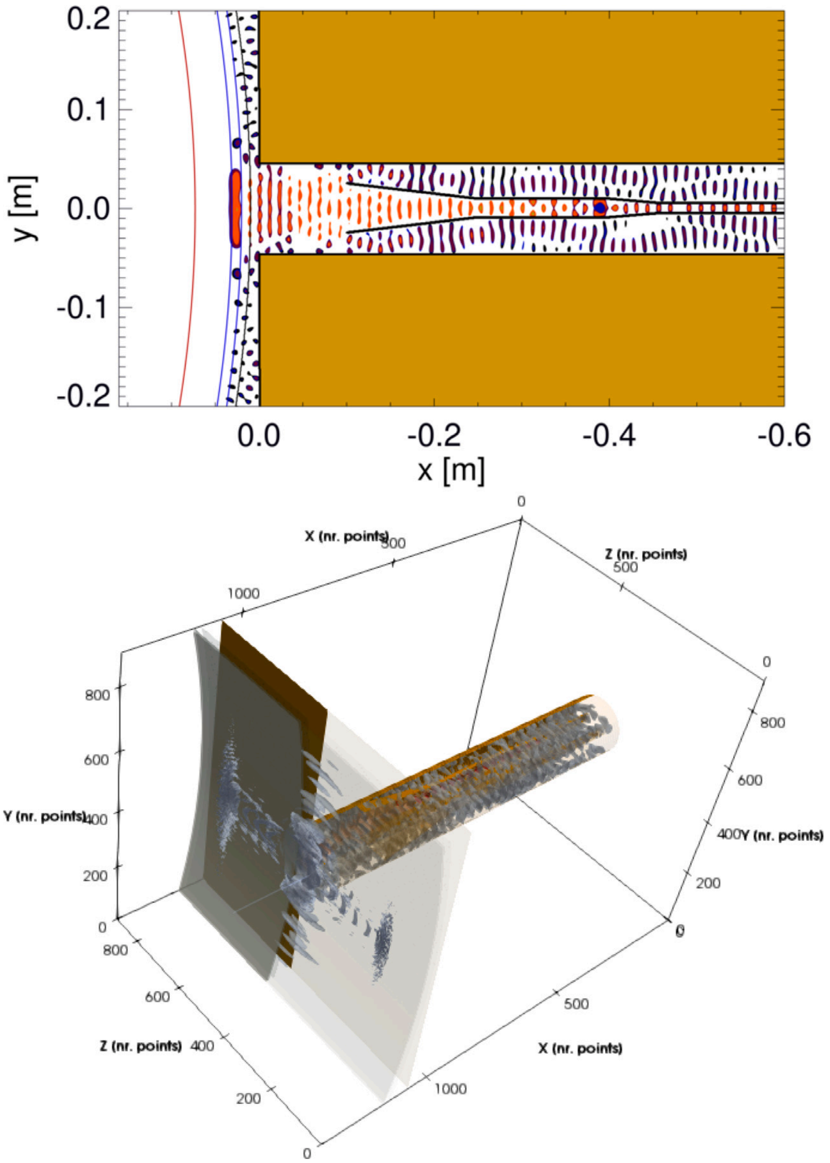

Fig. 2. On top, a snapshot of the 2D K band simulation taken at a frequency of $f = 18\,\text{GHz}$. On the bottom, a 3D simulation of the same problem.

investigate the physics of RF wave propagation in the electron cyclotron frequency range in magnetized plasmas [39].

Finally, a code originally designed for reflectometry simulation, such as those belonging to the REFMUL* family, can be applied to other areas as is, or with minute modification. For instance, REFMUL has been used to simulate a double vacuum window made of high-density polyethylene [40]. It has also been used for atmospheric entry applications, like the simulation of an electromagnetic environment for the RAM-C II flight experiment, obtained through a CFD code coupled to an electromagnetic propagation code [41]. A final example refers to its use in the study of beam broadening in the edge turbulent plasma of fusion machines for electron cyclotron resonance heating [42].

CRediT authorship contribution statement

F. da Silva: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **S. Heuraux:** Conceptualization, Investigation, Methodology, Writing – original draft, Writing – review & editing. **T. Ribeiro:** Data curation, Software, Validation, Writing – original draft. **E. Ricardo:** Formal analysis, Investigation, Software, Validation. **J. Santos:** Formal analysis, Investigation, Software, Validation, Writing – review & editing. **A. Silva:** Formal analysis, Investigation. **J. Ferreira:** Formal analysis, Investigation. **J. Vicente:** Formal analysis, Investigation. **G. De Masi:** Validation. **O. Tudisco:** Validation. **R. Cavazzana:** Validation. **G. Marchiori:** Validation. **R. Luís:** Investigation. **Y. Nietiadi:** Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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