

Problem-Oriented Simulation Packages and Computational Infrastructure for Numerical Studies of Powerful Gyrotrons

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Abstract. Powerful gyrotrons are necessary as sources of strong microwaves for electron cyclotron resonance heating (ECRH) and electron cyclotron current drive (ECCD) of magnetically confined plasmas in various reactors (most notably ITER) for controlled thermonuclear fusion. Adequate physical models and efficient problem-oriented software packages are essential tools for numerical studies, analysis, optimization and computer-aided design (CAD) of such high-performance gyrotrons operating in a CW mode and delivering output power of the order of 1–2 MW. In this report we present the current status of our simulation tools (physical models, numerical codes, pre- and post-processing programs, etc.) as well as the computational infrastructure on which they are being developed, maintained and executed.

1. Introduction

The gyrotrons are fast-wave free-electron devices (gyromonotron oscillators) operating on a physical principle known as cyclotron resonance maser (CRM) instability and thus sometimes referred to as CRM. They are among the most powerful sources of coherent radiation working in a CW (continuous wave) mode in the millimetre and the sub-millimetre wavelength regions of the electromagnetic spectrum and have numerous applications in the physical research and in various technologies [1, 2]. Certainly the most notable one, however, is their usage in the systems for electron cyclotron resonance heating (ECRH) and electron cyclotron current drive (ECCD) of magnetically confined plasmas in reactors for controlled thermonuclear fusion (e.g., tokamaks as, for example, ITER and DEMO) [3]. In recent years, the gyrotrons for fusion have demonstrated a remarkable progress reaching megawatt levels of the output power at frequencies of 140–170 GHz in a long pulse operation [1]. Their computer-aided design (CAD) and optimization is based on numerical experiments carried out using problem-oriented software packages for simulation of different subsystems of the tube (e.g., the electron-optical system (EOS), resonant cavity, internal mode converter, and so forth), i.e., applying the decomposition principle. Such computer codes are actively developed worldwide (see, for example [4] and the references therein). In this paper, we present briefly and illustrate the current status of the



simulation tools that are being developed and maintained by our research team in the framework of the collaboration with the leading institutions of the European gyrotron consortium (EGYC), IHHM-KIT (Germany) and CRPP-EPFL (Switzerland). An outlook for the future work is given as well.

2. Simulation tools for numerical investigation and CAD of gyrotrons

The gyrotrons are complex vacuum tubes that consist of several subsystems (e.g., electron-optical system (EOS) that forms a helical electron beam, in which most of its energy is associated with the rotational motion of gyrating electrons, i.e., “pumped beam” with high pitch factor; electro-dynamical system with a resonant cavity where the interaction of the electron beam and the excited high-frequency electromagnetic field takes place; quasi-optical system for formation of well collimated wave beam and its coupling to the output window, etc.). Therefore, following a reductionist approach (decomposition principle) different physical models are used to describe different subsystems. For example, the formation of the electron beam in the EOS is simulated by fully relativistic self-consistent static or time-dependent physical models implemented in ray-tracing (trajectory analysis) or PIC (Particle in Cell) codes, respectively. Analogously, the interaction in the cavity resonator is described by physical models which can be linear, nonlinear, time-dependent, static, and so on. Such big variety of physical models (e.g., full-wave, quasi-optical or based on one or another diffraction theory) is characteristic also for the system responsible for mode conversion, transmission and coupling of the wave beam. All this explains the necessity to use a great number of computer codes, combined into problem-oriented software packages on the basis of their common functional assignment. Figure 1 shows the structure of our simulation tools, i.e., both the main problem-oriented packages and the computational platforms on which they are installed and used.

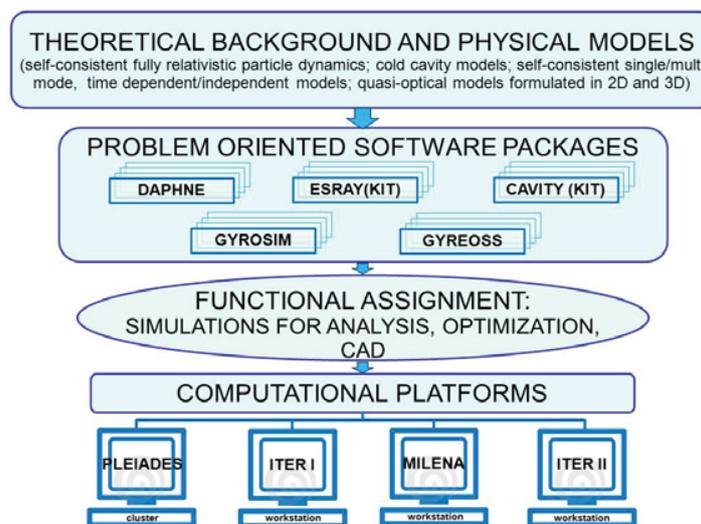


Figure 1. Simulation tools for numerical investigation, CAD and optimization of gyrotrons: problem-oriented software packages and computational infrastructure.

2.1. Current status and functionality of the problem-oriented software packages

Each problem-oriented package contains components (programs, subroutines, and so forth), from which the computational modules are built using appropriate numerical libraries and programming environments (IDE, compilers, debuggers). Some of them have a graphical user interface (GUI) and/or programs for pre-/post-processing and visualization of the results of numerical experiments. Below, these packages are annotated briefly.

2.1.1. *DAPHNE*

DAPHNE package [4] (developed at CRPP-EPFL) is a programming environment for optimization of EOS of gyrotrons. It is based on an adequate self-consistent physical model (formulated in 2.5D) which consists of a field part (a boundary value problem with Dirichlet and Neumann boundary conditions for the Poisson equation that governs the electrostatic potential distribution taking into account the space charge) and a dynamical part, which contains the relativistic equation of motion of charged macro particles representing the electrons of the beam. The computational region (2D meridional cross-section of an axially symmetric EOS) is discretized using a structured mesh with rectangular cells. DAPHNE is embedded in the ASTRID problem solving environment, which includes: a data base management system for memory and data handling (MEMCOM); 3D adaptive mesh generator; ASTRID finite element solver, graphic system for visualization, command language and interfacing modules. DAPHNE is implemented as a script written in ASTRID's command language and includes the two modules CFI (for calculation of the magnetic field of the coils of the tube) and PART (for integration of the equations of particles motion) written in FORTRAN. The script invokes both successively the particle pusher (PART) and the Poisson solver in an iterative loop until the process converges to a self-consistent solution.

2.1.2. *ESRAY (KIT)*

ESRAY (KIT) [5] is also a problem-oriented package for trajectory analysis (ray-tracing) of EOS based on a fully relativistic 2.5D electrostatic physical model. Its most characteristic distinguishing features are: (i) object-oriented program implementation in C++; (ii) advanced mesh generator which discretizes the computational domain with a great accuracy by structured boundary-fitted grids; (iii) versatile post-processing capabilities and visualization of all scalar and vector physical fields by colour maps; (iv) fast own solver for the boundary value problem by a finite difference method. The package consists of several modules: GRIDGEN (for geometry description and mesh generation), MAGGEN (for calculation the magnetic field of a system of solenoids), ESRAYS (for iterative solution of the self-consistent field problem), and OVIS. The latter module serves as a GUI and postprocessor that presents and visualizes the results of the simulation.

2.1.3. *CAVITY (KIT)*

The problem-oriented software package CAVITY (KIT) consists of a hierarchy of codes that begins with simple programs (e.g., for an analysis of the mode spectrum; cold cavity code, single mode self-consistent code) and culminates in the most sophisticated self-consistent multimode time-dependent code SELFT. Both the structure of the package and the physical models implemented in its modules has been reviewed recently [6]. The codes are written in FORTRAN and are invoked through a GUI. The GUI itself is in fact a Tcl/Tk script for a Linux (Unix) bash shell that controls: (i) the interaction with the codes, (ii) the specification of the input data, and (iii) the visualization of the results using a set of single commands in the menu window.

2.1.4. *GYROSIM*

GYROSIM is a problem-oriented software package which includes numerical libraries and source codes of various computational modules (standalone programs, subroutines, pre-, post-processing, and visualization codes) for solving a variety of problems pertinent to the simulation and CAD of gyrotrons using a rich set of adequate physical models [7]. Unlike other packages described above, it is not, however, specialized to only one subsystem of the gyrotron tube. Rather, the individual components of GYROSIM are designed for simulation of all main subsystems of the gyrotron tube, notably: (i) the electron-optical system (EOS), (ii) the magnetic system which includes the main magnet and an arrangement of additional coils, (iii) the electrodynamical system (resonant cavity), and (iv) the quasi-optical system for mode conversion and transmission of the radiation.

It should be mentioned that the codes for numerical modelling of the EOS (GUN-MIG/CUSP) are based on a 2.5D physical model, which is analogous to the one implemented in DAPHNE and ESRAY

and therefore provide results that are consistent and in a good agreement with each other. Besides the differences in their program implementation, GUN-MIG/CUSP, however, allows magnetron injection guns (MIG) with a reversal of the magnetic field (e.g., a magnetic cusp) that form axis-encircling (aka uniaxial) beams to be simulated with an increased accuracy. Similarly, the codes of GYROSIM for simulation of the electro-dynamical system cover the same functionality as the CAVITY (KIT). At the same time, there are some notable differences between them. For instance, the CAVITY (KIT) can treat both conventional and coaxial resonators but at fundamental operation while the cavity codes belonging to GYROSIM are specialized only to cavities without an insert but can simulate operation at the second (and in the case of a large orbit gyrotron (LOG) even higher) harmonics of the cyclotron frequency. In its current form, the GYROSIM is a heterogeneous package and includes components written in different languages (Fortran 77, Fortran 90, C, C++, SciLab, and so on), operational and/or portable to different computational platforms (ranging from laptops and workstations to mainframe and supercomputers), and executable under different (genuine as well as emulated/virtualized) operating systems (e.g., Unix, Linux, Windows, Cygwin). Another characteristic feature of the package is that it is being built following a concept of extensibility which allows us to add/replace easily different computational modules and in such a way to modify both the numerical algorithms and the physical models implemented in the programs. The latest upgrade of GYROSIM package has been carried out in parallel with the development of a novel module called GO&ART (which stands for Geometric Optics and Analytic Ray Tracing). It consists of several codes (RAYS, COMODES, and TRACE) for analysis of quasi-optical components (Vlasov and Denisov type launchers, reflectors and phase-correcting mirrors, and so on) as well as systems based on them (e.g., internal mode converters and transmission lines). As an illustration, some screenshots of these programs are shown in figure 2.

2.1.5. GYREOSS

Initially, GYREOSS has been conceived as a package of codes for simulation of EOS using a physical model formulated in three space dimensions in order to take into account the departure from axial symmetry due to various misalignments (for instance of the electrodes, of the magnetic coils, etc.) and non-uniformities. Its initial version has been implemented using the gmsh package for meshing, pre- and post-processing and GetDP as a solver [8]. In the recent years, however, GYREOSS has evolved as a test bench for experimenting with different numerical methods, solvers and algorithms in 3D aiming the final goal – a parallel 3D code for numerical simulation and CAD of EOS of gyrotrons.

The latest version of GYREOSS is being developed using the FreeFEM++ problem solving environment [9]. Recently a series of experiments have been carried out in order to study both the accuracy and the speed of several experimental electrostatic solvers of GYREOS based on different Finite Element Method's (FEM) formulations and various combinations of finite elements (e.g., the Raviart–Thomas finite elements, real-time three-dimensional (RT3d) vector-valued $H(\text{div})$ -conforming finite elements, and continuous piece-wise linear finite elements P03) and a method for solving the resulting set of linear equations. These studies are being complimented by investigations focused on the optimization of the used tetrahedral meshes and their adaptive refinement (AMR) using the Hessian of the solution. At the same time, a preparation for a MPI parallelization of the code is in progress now.

A screenshot that illustrates the GUI and the visualization (based on the medit – an interactive mesh visualization software [10]) used by GYREOSS is shown in figure 3.

2.2. Available computational platforms for code maintenance and development

All packages outlined above (CAVITY, ESRAY, GYROSIM, GYREOSS) are installed and are operational on the workstations of the Bulgarian research team (see figure 1), except DAPHNE, which is available to us for remote execution and maintenance on the PLEIADES2 cluster from Sofia. Since the outstanding performance of PLEIADES2 is well known, we will mention only the basic characteristics of the most powerful of our workstations. ITER I has two CPU AMD Opteron™ Dual Core 275, 2.2 GHz and RAM 4 GB DDRAM with a MB Supermicro-Dual Opteron and SVGA Nvidia

3. Conclusion

The problem-oriented packages outlined in the previous section are under continuous development and improvement. Recently they have been used in a series of numerical experiments, carried out to study the designs of powerful gyrotrons that are under consideration and/or development at present [5]. The conducted simulations give a deeper physical insight into the operation of high-performance gyrotrons of megawatt class and are good benchmarks that demonstrate the improved capabilities and functionality of the upgraded codes. Moreover, these results suggest some further experiments for more detailed study of the correlation between the beam-quality parameters and efficiency, on one hand, and the particular design (configuration of the electrodes, tailoring of the magnetic field, etc.), on the other hand. It is expected that the novel and upgraded versions of the simulation packages will contribute to the development of the next generation of powerful gyrotrons for fusion with an improved performance.

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