Modelling, simulation and computer-aided design (CAD) of gyrotrons for novel applications in the high-power terahertz science and technologies

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Abstract. Gyrotrons are the most powerful sources of CW coherent radiation in the sub-THz and THz frequency bands. In recent years, they have demonstrated a remarkable potential for bridging the so-called THz-gap in the electromagnetic spectrum and opened the road to many novel applications of the terahertz waves. Among them are various advanced spectroscopic techniques (e.g., ESR and DNP-NMR), plasma physics and fusion research, materials processing and characterization, imaging and inspection, new medical technologies and biological studies. In this paper, we review briefly the current status of the research in this broad field and present our problem-oriented software packages developed recently for numerical analysis, computer-aided design (CAD) and optimization of gyrotrons.

1. Introduction
The family of gyro-devices includes both amplifiers (e.g., gyro-klystrons, gyro-TWT) and oscillators (gyrotron, aka, gyro-monotron, gyro-BWO, etc.). In fact, they are fast-wave free-electron vacuum tubes in which an annular beam of electrons gyrates (thus the prefix “gyro” in their names) following helical orbits and interacts with the high-frequency field having a phase velocity exceeding the speed of light in the resonant structure (cavity). Unlike the slow-wave Cherenkov devices (for example BWO, TWT) the dimensions of the resonant structure (e.g., cavity radius $R_{\text{cav}}$) can be much larger than the wavelength of the generated radiation. This allows powerful electron beams (formed by an electron-optical system (EOS) with a magnetron-injection gun (MIG) and an adiabatically increasing magnetic field provided by a superconducting magnet) to be injected into the cavity, where the electrons exercise rotational motion with a cyclotron frequency $\Omega_c = \frac{eB}{mc}$ on a circle with a Larmor radius $r_L = \frac{v_{\perp}}{\Omega_c}$. Here $\frac{e}{m}$ is the electron charge-to-mass ratio, $B$ is the magnetic field strength

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and $v_\perp$ is the transverse (rotational) velocity. In the resonator, where $B$ attains its maximum value, most of the energy of the electrons is associated with their rotational motion and the velocity pitch factor $\alpha = \frac{v_\perp}{v_z} > 1$, $v_z$ being the axial velocity. During the interaction of the electrons with the transverse electric field, some electrons lose energy to the wave, while others gain energy. Due to the relativistic dependence of the electron mass $m = m_0\gamma$ on the energy $E$ ($m_0$ and $\gamma = E/m_0c^2$ being the rest mass and the relativistic Lorenz factor, respectively, and $c$ is the speed of light), the cyclotron frequency also changes accordingly (i.e., increases for deaccelerated electrons and decreases for accelerated ones) leading to a non-isochronous circular motion, which results in an azimuthal bunching of the electrons. This mechanism is responsible for an efficient beam-wave interaction with a positive gain at the cyclotron resonance provided that proper synchronization conditions are satisfied. Such resonance occurs at a frequency $\omega = s\Omega_c + v_z k_z$, where $s$ and $k_z$ are the harmonic number and the axial wave number, respectively. The gyrotrons are distinguished from other gyro-devices by the fact that they operate at frequencies close to the cut-off frequency of the cavity ($\omega_{cut} = c \frac{\chi_{mn}}{r_{cav}}$) where $\chi_{mn}$ is the n-th zero of the Bessel function $J_m$ for TM modes and of its derivative $J'_m$ for the TE modes), i.e. the Doppler shift term $v_z k_z$ is negligibly small and thus $\omega \approx s\Omega_c$ [1]. A helpful engineering estimate gives for the fundamental resonances ($s=1$) approximately 28 GHz per 1 T. In recent years, the progress in the development of superconducting magnets that deliver field intensity up to 20 T and the operation at higher harmonics of the cyclotron frequency have facilitated the advancement of the gyrotrons from the sub-THz to the THz range. At present, they are the most powerful sources of CW coherent radiation in this region of the electromagnetic spectrum and contribute to bridging the so-called THz gap [2, 3]. The remarkable breakthroughs demonstrated by them, alongside with the significant improvement in their operational performance utilizing more compact cryo-free superconducting magnets, not only increased their number in many traditional fields, but have also opened an avenue to many novel and prospective applications in the fundamental physical research and most notably in the emerging high-power terahertz science and technology [4–7].

Although all gyrotrons operate on the same principle (known as electron cyclotron resonance maser (ECRM) instability) and can be described in the framework of a unified approach using identical physical models, each particular application imposes specific requirements to the operational output parameters and sets some constructive restraints. In order to elucidate them, first, we present briefly (Sect. 2) the most prominent applications of the gyrotrons. Then, in Sect. 3 we depict our tools (computational infrastructure, problem-oriented software packages and stand-alone codes) developed by us for numerical analysis, computer-aided design (CAD), and optimization of powerful gyrotrons for fusion research and sub-THz gyrotrons for various advanced spectroscopic techniques, materials processing, and novel medical technologies. We conclude the paper with an outlook on the envisaged future work in this field.

2. Traditional, novel, and prospective applications of the gyrotrons

The advantages mentioned above (most notably the unprecedented output power in the sub-THz to the THz frequency range in CW mode) makes the gyrotrons versatile and appropriate radiation sources for many physical studies and technological processes. Some of the most prominent traditional, novel and prospective applications are represented as branches of an ever-growing tree in figure 1. Among the traditional and most matured applications is their usage for electron cyclotron resonance heating (ECRH) and current drive (ECCD) of magnetically confined plasma in various reactors (e.g. tokamaks and stellarators) for controlled thermonuclear fusion. The gyrotrons are used also for plasma initiation (start-up), plasma control (suppression of the neo-classical tearing modes) and for plasma diagnostics based on a CTS (collective Thomson scattering). The 170-GHz gyrotrons developed in Japan, the EU and the Russian Federation have demonstrated megawatt levels of the output power with an efficiency exceeding 50% at long pulse operation (3600 s) and have reached the requirements of ITER [1]. The next big step in the fusion research – DEMO, however, requires even higher frequency, power and efficiency (230 GHz, 1.5 MW, and 60%, respectively) and, additionally,
multi-frequency operation. Compared with other tubes, the gyrotrons for fusion use higher beam currents, highly oversized cavities, and larger emitters. This makes the influence of such factors as space-charge effects, beam instabilities, nonuniformity of the emission, misalignment and thermal shift of the electrodes, etc., more severe. Since most of these effects are both non-stationary and non-axially symmetric they could be taken into account using time-dependent self-consistent physical models formulated in three dimensions (3D) and implemented in 3D numerical codes.

Figure 1. The tree of gyrotron applications.

In the field of plasma physics, the gyrotrons are used for studies on various gas discharges initiated by microwaves. A good example is also the Electron Cyclotron Ion Source (ECIS) for production of multi-charged ion beams. One of the newest applications proposed recently is the remote detection of concealed radioactive materials. In this promising technique, a focused beam of THz radiation initiates an avalanche breakdown provided seed electrons (produced by the ionization radiation) are present.

The gyrotrons are used as sources of coherent CW sub-THz radiation in a number of advanced and precise spectroscopic methods. Among them are ESR (Electron Spin Resonance) spectroscopy, and DNP-NMR (Nuclear Magnetic Resonance with a signal enhancement through Dynamic Nuclear Polarization) [5–8]. The latter technique is revolutionizing the studies of proteins and other biomolecules offering significant reduction of the spectra acquisition time and an increased sensitivity. Its variety, the solid-state DNP-NMR, is a powerful method for studies on the molecular structure and surface characterization of many different materials. Another novel spectroscopy is based on the X-ray detected magnetic resonance (XDMR). In this element and edge-selective pump and probe technique, the X-ray magnetic circular dichroism is used to probe the resonant precision of the magnetization components in an intense field of a sub-THz wave produced by a gyrotron. XDMR spectroscopy is a unique tool for studies on the magnetization dynamics induced by the precision of both the spin and orbital moments. The newest high-precision spectroscopy that uses a gyrotron as a radiation source has been developed quite recently for a direct measurement of the ground state hyperfine splitting.
(HFS) of the positronium (Ps). Recently, the whole Breit–Wigner resonance of the stimulated transition from o-Ps to p-Ps has been measured for the first time using a frequency tunable gyrotron in the range 201 GHz to 205 GHz. In the Research Center for Development of Far-Infrared Region at the University of Fukui, Japan many gyrotrons have been developed for the above mentioned spectroscopic studies [5–7].

When irradiated by sub-THz and THz waves, many substances acquire unique characteristic spectra (“fingerprints”) that are used for materials identification and characterization, as well as for a security control.

Thermal treatment of advanced materials (e.g., ceramic sintering) using mm-wave radiation of gyrotrons is a mature industrial grade technology. It benefits from the well-known advantageous features of the microwave heating: (i) uniform volumetric and selective heating; (ii) rapid heat transfer and high heating rate from several hundred to thousands of degrees per second; (iii) precise control of the absorbed energy; (iii) lower losses and higher efficiency compared to other heating methods. Usually, the process is carried out inside an applicator in which steerable mirrors and reflectors are used for an additional homogenization of the microwave irradiation. The gyrotrons are used in industrial facilities for microwave melting, joining and sealing of glass; thermal processing of semiconductors; annealing of thin Si films for solar cells; polymer coating, molding, and curing; drying of porous materials, etc. (visit: http://www.gyrotrontech.com). The radiation of gyrotrons is promising also for several emerging technologies (most notably for MAS, microwave assisted synthesis) where both thermal and non-thermal effects are used.

Recently, several concepts of novel medical technologies utilizing gyrotron radiation have been developed. Among them is the local hyperthermia of cancerous tumors. As more promising, however, we consider its combinations with other methods that, hopefully, would instigate a synergy effect of the combined treatment. One of them is a hybrid dual-beam therapy, which combines the BNCT (boron neutron capture therapy) with hyperthermia by sub-THz wave irradiation [9]. The other hybrid technique combines such hyperthermia with photodynamic laser therapy (PDT) [10].

The gyrotrons have demonstrated a great potential for the development of many high-power terahertz technologies in other fields as well. For example, in the next generation mm-wave communications, advanced radars, nonlethal weapons (e.g. active denial systems), energy transmission (beaming) and even microwave rocket propulsion, just to name a few due to the limited space here. We anticipate that in the near future many other novel applications of sub-THz and THz gyrotrons will emerge.

3. Development of problem-oriented software packages for numerical studies, computer-aided design (CAD) and optimization of gyrotrons
Motivated by our involvement in the development, study, and utilization of gyrotrons for several of the above-mentioned application, in recent years we have built a hierarchy of modeling and simulation tools (see figure 2) that are being used for CAD of high-performance tubes. Our approach encompasses all levels of that hierarchy starting from the formulation of adequate physical models and selection of efficient numerical methods, programming libraries, and appropriate integrated development environments (IDE). Then, the mathematical formulations of the physical models are being implemented (coded) in computational modules, subroutines and other programing building blocks of our problem-oriented (i.e., specialized to different subsystems of the device) software packages and several stand-alone computer programs. Both the development (programming, debugging, benchmarking) and the numerical experiments are being carried out using the available computational infrastructure that consists of several workstations.

The structure of the developed software tools used for numerical studies and CAD of gyrotrons is presented in figure 3. Also shown here is the functional assignment of their components (computational modules) to the iterative design loop (bottom panel of the figure).
Figure 2. Hierarchy of the modelling and simulation tools.

Figure 3. Structure of the software tools and their functional assignment to the iterative CAD.

The problem-oriented software package GYROSIM (an abbreviation from GYROtron SIMulation) contains computer codes for numerical analysis and CAD of three of the most important subsystems of the gyrotron tube, namely the EOS (including a MIG and a set of magnetic coils), the resonance cavity (electro-dynamical system), and the quasi-optical system. An important task during the initial design is the selection of an appropriate operating cavity mode and preliminary analysis of the operational parameters (beam voltage and current, velocity ratio (pitch factor), magnetic field intensity) while iterating different configurations and sizes of the resonant structure. On this stage, several programs (EIGEN, BMOD) for analysis of the cavity spectrum and scanning of the corresponding resonances are used. Furthermore, the codes IS and QFAC are used for an initial evaluation of the starting beam currents (based on the linear gyrotron theory) and the Q-factors (diffractive, Ohmic and loaded), respectively. This is followed by simulations carried out using cold-cavity and single-mode static (time-independent) codes (CCC_CAV, CS-SMTI) for simulation of the beam-wave interaction and for a preliminary estimation of the possible operational parameters (output power, efficiency, etc.). After
the initial design, an iterative design loop starts, during which more sophisticated (based on self-consistent time-dependent multimode physical models) codes CS-MMTD are used.

GYROSIM contains two codes for CAD of the EOS, namely GUN-MIG and GUN-CUSP. In both of them self-consistent fully relativistic physical models that take into account the space-charge and initial velocity spread are used. They are formulated in 2.5D, i.e. in a 5D phase space of two spatial and three momentum coordinates in an axially-symmetric coordinate system. Their field solvers are based on the finite-difference method (FDM) with a successive over relaxation and an automatic selection of an optimal parameter of the relaxation. GUN-MIG is used for an analysis of conventional MIGs that form helical electron beams, in which the guiding centers of the electron orbits are off-axis. MIG-CUSP is specialized to EOS with a field reversal that form axis-encircling (aka uniaxial) beams that are used in the Large Orbit Gyrotrons (LOG). These codes for trajectory analysis (ray tracing) include auxiliary programs for calculation of the magnetic field distribution generated by a set of solenoids (together with the main superconducting coils) as well as for post-processing and visualization of the results of the numerical experiments.

Many applications of the gyrotrons require a well-collimated wave beam. In order to transform the wave of the high-order operating mode into a Gaussian-like beam an internal mode converter is used. It includes a launcher of either Vlasov or Denisov type and a system of mirrors that shape the output radiation before coupling it to the vacuum window. The module GO&ART (which stands for Geometric Optics and Analytical Ray Tracing) of the GYROSIM package has several codes (RAYS, COMODES, and TRACE) for CAD of such quasi-optical system. The code RAYS uses the analytical theory for designing Vlasov type antennas, while COMODES utilizes a model based on the coupled modes theory and is used for an analysis of dimpled-wall launchers (Denisov launchers). The system of reflectors and phase correcting mirrors is designed using the code TRACE.

Novel modules added recently to GYROSIM have been used for a numerical study on finite-bandwidth resonances of high-order axial modes (HOAM) in a gyrotron cavity [11]. The proposed approach allows one to study the frequency response of the cavity using different resonance curves obtained from the solution of the inhomogeneous Helmholtz equation for the field amplitude by the finite-difference method (FDM). The results give deeper insight into the continuous frequency tunability through excitation of a sequence of HOAM. As an illustration, in figure 4 we present the calculated axial field profiles of such sequence for the operating mode TE₄₃₁.

![Figure 4](image)

**Figure 4.** Configuration of the gyrotron cavity studied and field pattern of the TE₄₃₁ mode (upper panel); and axial profiles of the field intensity for a sequence of HOM (lower panel). Here \( f/f_{\text{cut}} \) is the frequency normalized to the cut-off frequency of the cavity.
As already mentioned, the departure from axial symmetry due to various inevitable misalignments and nonuniformities (for instance nonuniformity of the emission) requires the utilization of physical models formulated in 3D. In order to meet this challenge, we have started the development of the problem–oriented package GYREOSS (GYREOSS stands for Gyrotron Electron-Optical System Simulation) [12]. This PIC (particle-in-cell) code is implemented as a library of scripts for the partial differential equations solver FreeFEM++ [13] and uses its IDE FreeFEM++-cs for the code development and execution. The computational domain is discretized by unstructured tetrahedral grids produced by gmsh [14] or by the mesh generator embedded in FreeFEM++. The Poisson equation for the potential of the electric field is solved by the finite element method (FEM). The field produced by the coils of the magnetic system is calculated using a paraxial expansion of the magnetic field along the axis of the tube. For scattering (allocation) of the space charge to the mesh an efficient and fast charge-conserving algorithm is used. In the relativistic particle pusher of GYREOSS, a second-order leap-frog Boris–Buneman scheme for tracing the motion of the particles is implemented. The code uses the advanced visualization capabilities of FreeFRM++-cs for post processing and analysis of the results of the numerical experiments. As an illustration, figure 5 shows a screenshot from the simulation of a coaxial gyrotron for plasma heating (2 MW at 170 GHz). A work on the parallelization of the current serial version of GYREOSS package will be the next step in its development.

Figure 5. Screenshot taken during the simulation of a coaxial gyrotron for ECRH and ECCD.

4. Conclusions
The developed tools for modelling and simulation of gyrotrons have been used successfully for CAD, numerical studies, and optimization of the operational performance of a series of radiation sources for various applications presented briefly in this paper. Most of them have been constructed and manufactured at the Research Center for Development of Far-Infrared Region (FIR-UF) and are being currently used for advanced spectroscopic techniques (ESR, DNP-NMR, XDMR, measurement of the HFS of positronium), materials processing, novel medical technologies, etc. The reach set of computer codes integrated into the problem-oriented packages GYROSIM and GYREOSS is a solid base for further numerical studies and CAD of powerful gyrotrons many anticipated novel applications.

Besides the ongoing continuous work on the improvement of the program implementation, testing and benchmarking of the computational modules, upgrade of the underlying programming libraries, and so on, we plan a further extension of these packages adding new components that will take into
account more physical factors. Among them are, for instance: the influence of the trapped (reflected) electrons; the impact ionization of the ambient high vacuum atmosphere in the tube by the beam electrons (and, thus, resulting space charge compensation); various instabilities (e.g. diocotron instability, electrostatic Bernstein instability, Langmuir instability, electrostatic cyclotron instability (aka negative-mass instability), trapped electron instabilities and others) affecting the beam formation and the beam-wave interaction.

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