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# Report on the computer code and simulation tools which will be used for RF power unit design and cost optimization

W. Wuensch[1)*], M. Diomede[†], A. Gallo[†], D. Alesini[†], C. Rossi[*], A. Cross[‡], L. Zhang[‡], L. Nix[‡], X. Wu[*]

On behalf of the CompactLight Partnership

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[*] CERN, Switzerland, [†] INFN, Italy, [‡] Strathclyde, United Kingdom

[1] Corresponding author: walter.wuensch@cern.ch

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# Abstract

A central element in designing CompactLight is a global optimization that takes into account the performances and costs of the different parts of the facility; injector, linac and photon production. Each of these different areas is individually highly complex, and there are many interconnections. This deliverable report describes the array key computer-based tools which have been assembled and developed for use in the optimization of the CompactLight linac This report describes the array of key computer tools which have been put into place in order to carry out the design, simulation and optimization of the CompactLight linac as well as some preliminary results.

# Contents

# 1 Introduction

The CompactLight project seeks to bring together many new developments in accelerator technology, simulation tools and photon science with the objective of producing a comprehensive design of new-generation XFEL facility with significantly smaller footprint and lower cost than existing facilities.

A central element in achieving this goal for CompactLight is a design process which is centred on a global optimisation that takes into account the performances and costs of the different parts of the facility; injector, linac and photon production. Each of these different areas is individually highly complex, and there are many interconnections. A global optimisation must consequently take into account a large number of parameters, which means that a computer-based optimisation procedure must be put into place.

This deliverable report describes the key computer-based tools which have been assembled and developed for use in the optimisation of the CompactLight linac.

The linac of CompactLight represents a major part of the overall facility cost and is the focus of WP4. The linac begins at the output of the injector where the beam is fully relativistic, with an energy of 300 MeV, and ends when the beam has achieved its final energy, in the range from 4.5 to 6 GeV. In fact the final energy is one of the important parameters which must be determined by the global optimisation. The linac is composed of repeated modules, each with an identical layout and composition. The key components of the module RF system are the modulator, klystron, pulse compressor, waveguide network and accelerating structure. The module also includes diagnostics, magnetic elements such as focusing quadrupoles and correcting dipoles as well as sub-systems such as vacuum and cooling.

The elements of the module will all be developed and optimised using simulation tools in such a way that important parameters can be scanned and the results recorded in order to be used in higher level optimisation. This report follows with three sections each describing an important group of simulation and optimisation tools:

- **Module RF system simulation** - This covers the RF power source, pulse compression parameters, waveguide system performance and accelerating structure. Dimensions and RF performances are determined.
- **Project Breakdown Structure (PBS) for the linac** - This organises the system hardware, provides an efficient means of documentation and exchange of parameters. It will in later stages also be used to provide data for costing.
- **Gyroklystron, linearizer pulse compressor, and waveguide system: RF design and beam tracking tools** - Although the gyroklystron is used in the lineariser system, which is in the injector, the power source development is included in the mandate for WP4, due to technical similarity and overlap of expertise.

# 2 Module RF system simulation

## 2.1 Introduction

WP4 will define the RF system for the main linac of the FEL facility in the main and sub-design variants. A key goal will be to define a standardised RF unit which can be used in all main and sub-design variants. Making a standardised design available can simplify the preparation of future construction projects, stimulate the industrialisation process and provide cost savings for future facilities.

Goal of this task is to develop the design tools needed to provide input for the global optimisation done in WP2.

In WP4, one of the goals is to perform the electromagnetic (EM) design of the energy booster in X-band. The booster is based on several Travelling Wave Accelerating Structures (TWASs) fed by klystrons and pulse compressor systems. By using pulse compressor schemes, one klystron can be able to feed several structures through a waveguide network. Thus, the booster can be composed by a sequence of RF modules, each one composed by a certain number of structures.

Parameters to be determined are: the structure length, the irises tapered profile in the structure, the total number of klystrons and pulse compressors, the number of structures, klystrons and pulse compressors per module.

The goal is to maximise the RF efficiency, i.e. minimise the total number of klystrons. The key parameter to be maximised is the TWAS effective shunt impedance assumed as the RF efficiency figure of a structure.

Input from WP2 is the average accelerating gradient, which defines the compactness of the machine. Input from WP6 is the average iris radius of the structure, which strongly affects the beam stability.

## 2.2 General approach

The workflow we used for the optimization procedure is the following:

1. Chose a reference value of the accelerating field (input from WP2);
2. Define the RF pulse compressor characteristics;
3. Set the average iris radius (input from WP6);
4. Electromagnetic design and optimization of the regular cell;
5. Find the highest structure effective shunt impedance by scanning the total length and the iris tapering to reduce the total number of power sources;
6. Verify the peak modified Poynting vector value at the nominal gradient;
7. Design a realistic RF module on the basis of the final energy and existing klystrons: power distribution network;
8. Finalise the electromagnetic design: input and output couplers;
9. Perform an EM simulation of the entire structure with couplers for a fine tuning procedure. The field maps will be passed to WP6 for beam dynamics simulations.

Iterations cycles along the defined procedure are required, as a consequence of discussions and data exchange with other WPs. The same approach has been used for several projects at INFN-LNF: SPARC_LAB [1], ELI-NP [2], EuPRAXIA@SPARC_LAB [3].

## 2.3 Software tools

For the design and optimization procedure we used two commercial computer codes: HFSS and MATLAB.

HFSS (High Frequency Structure Simulator) is a finite element method solver for electromagnetic structures from ANSYS. It is a 3D electromagnetic simulation software for designing and simulating high-frequency electronic products such as antennas, antenna arrays, RF or microwave components, high-speed interconnects, filters, connectors, IC packages and printed circuit boards [4].

MATLAB (matrix laboratory) is a multi-paradigm numerical computing environment and proprietary programming language developed by MathWorks. MATLAB allows matrix manipulations, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other languages, including C, C++, C#, Java, Fortran and Python [5].

We use HFSS to design the structure's single cell and calculate the EM fields and the main RF parameters like shunt impedance, q-factor, group velocity, modified Poynting vector. In Fig. 1 a sketch of the cell geometry for EuPRAXIA@SPARC_LAB is reported [6], [7]. It is a double rounded cell with an elliptical profile of the iris. In Fig. 2, the related RF parameters, as a function of the iris radius of the cell, are shown. The goal is to optimise the geometrical dimensions $r_0$, $t$ and $r_2/r_1$ in order to increase the shunt impedance and minimise the modified Poynting vector.

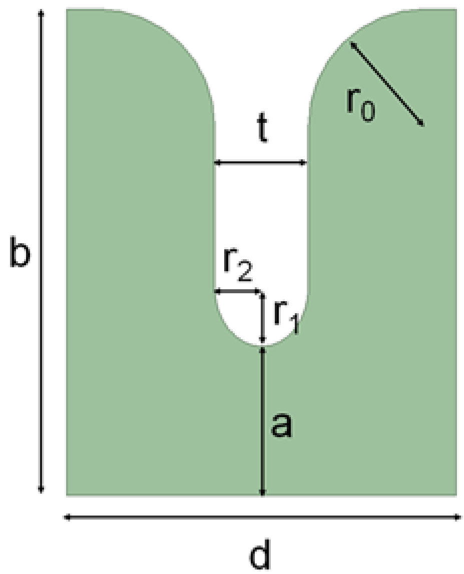


Figure 1: Sketch of a cell geometry

On the base of the parametrised specs of the basic cell provided by HFSS, we use MATLAB to calculate the main RF and geometrical parameters of an accelerating structure modelled as a stack of basic cells with tapered iris radius. These parameters are: effective shunt impedance, peak value of modified Poynting vector, total length, filling time, cell-by-cell iris modulation, external quality factor of the SLED. By using analytical formulas, it is possible to calculate these parameters for particular cases like constant impedance and (with some approximation) constant gradient structures. Fig. 3 shows the typical output of a SLED while Fig. 4 shows the

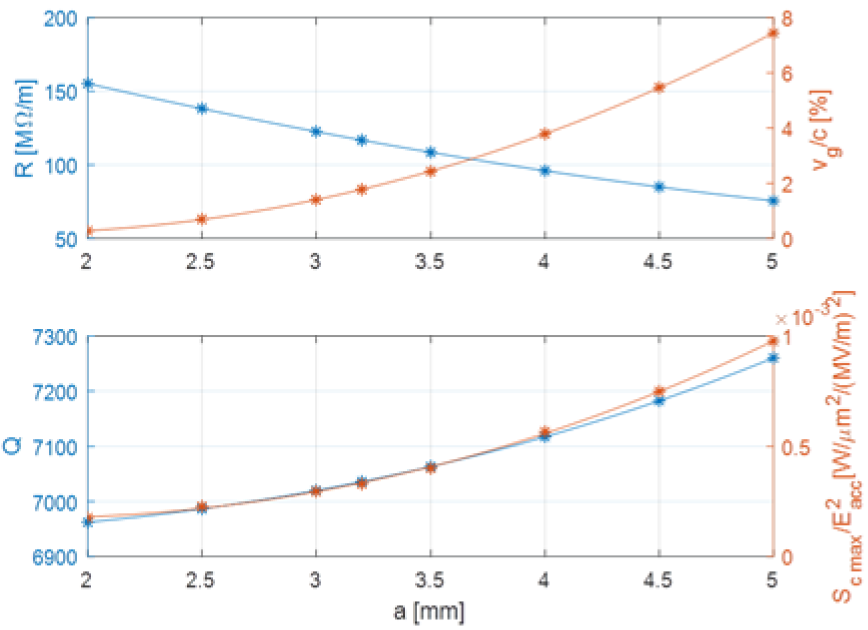


Figure 2: Main cell parameters as a function of the iris radius

comparison between a constant impedance and a constant gradient structure calculated for EuPRAXIA@SPARC_LAB.

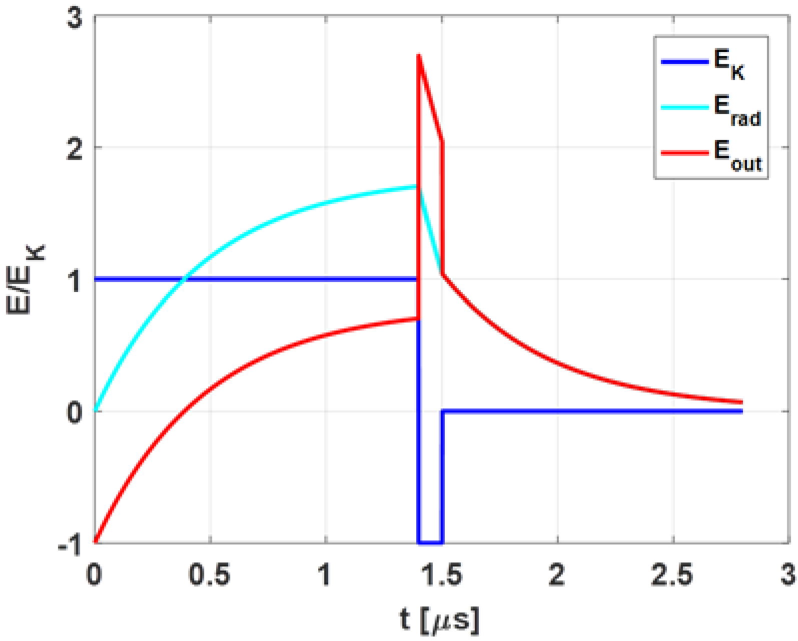


Figure 3: Typical output of a SLED

Generally, a constant impedance structure is not the best solution in terms of breakdown rate, while the analytical solution of constant gradient structures considers the approximation of R/Q constant along the propagation axis and the results are valid only in a steady state. Considering these facts, we developed MATLAB code that implements main formulas of trav-

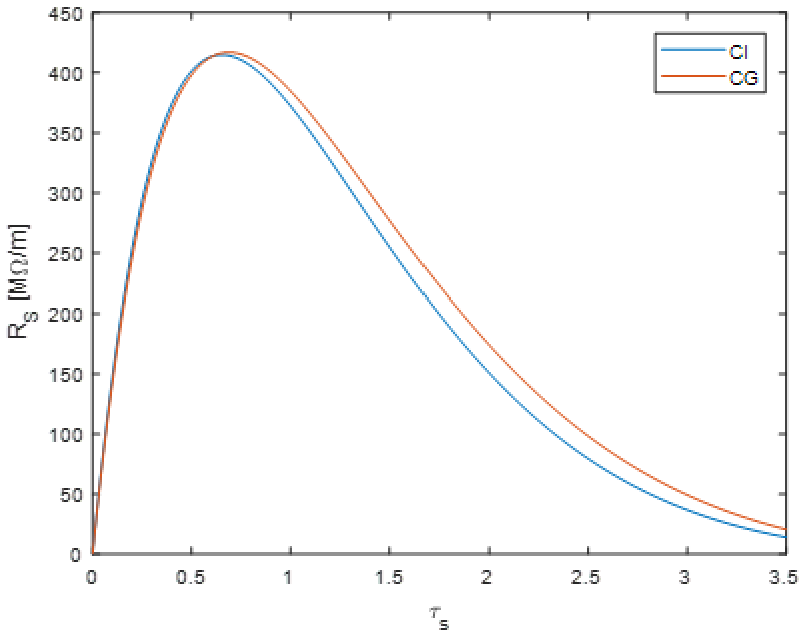


Figure 4: Effective shunt impedance of constant impedance and constant gradient structures as a function of the section attenuation

elling wave structures without approximation using as an input the RF parameters calculated with HFSS. In this way, it is possible to calculate the parameters of structures with an arbitrary cell-by-cell iris modulation. For simplicity, the code considers a linear iris modulation and calculates the structure parameters for different structure lengths and iris tapering slopes. Constant impedance and constant gradient results are used as a guideline of this numerical approach. Considerations about the power distribution system (i.e. number of structures per klystron) and expected breakdown rate allows the optimal structure length and tapering slope to be chosen. The goal of this optimisation process is to maximise the effective shunt impedance keeping under control the modified pointing vector. In Fig. 5, effective shunt impedance as a function of the tapering angle for three structure lengths is shown, while in Fig. 6 the peak value of modified Poynting vector is shown (from EuPRAXIA@SPARC_LAB TDR).

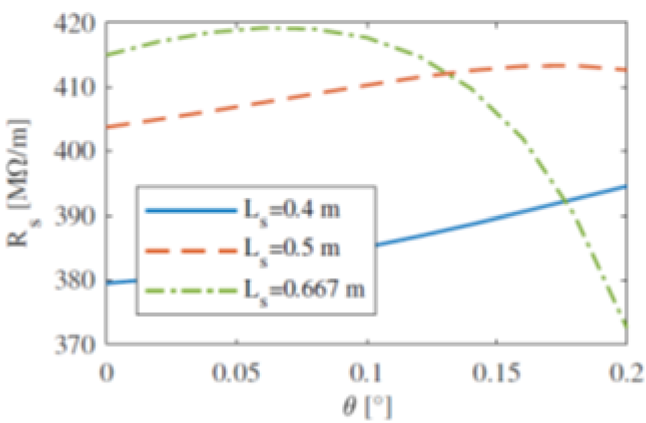


Figure 5: Effective shunt impedance as a function of the tapering angle for three lengths of the structure

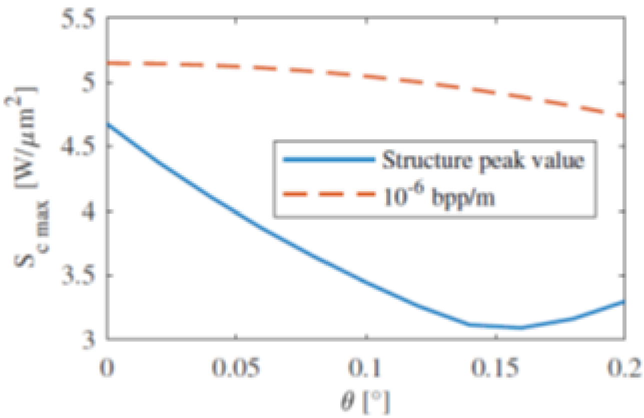


Figure 6: Modified Poynting vector as a function of the tapering angle for a fixed length of the structure

Once the design of the cells has been determined, we need to go back to HFSS to design the input and output power couplers. The goal is to minimise reflection coefficient, pulsed heating and multipolar components of the magnetic field. An input for the simulations is the RF input power calculated with MATLAB. In Fig. 7, the design of input and output couplers with the related superficial magnetic field of the C-band structures for the ELI-NP project are shown [8].

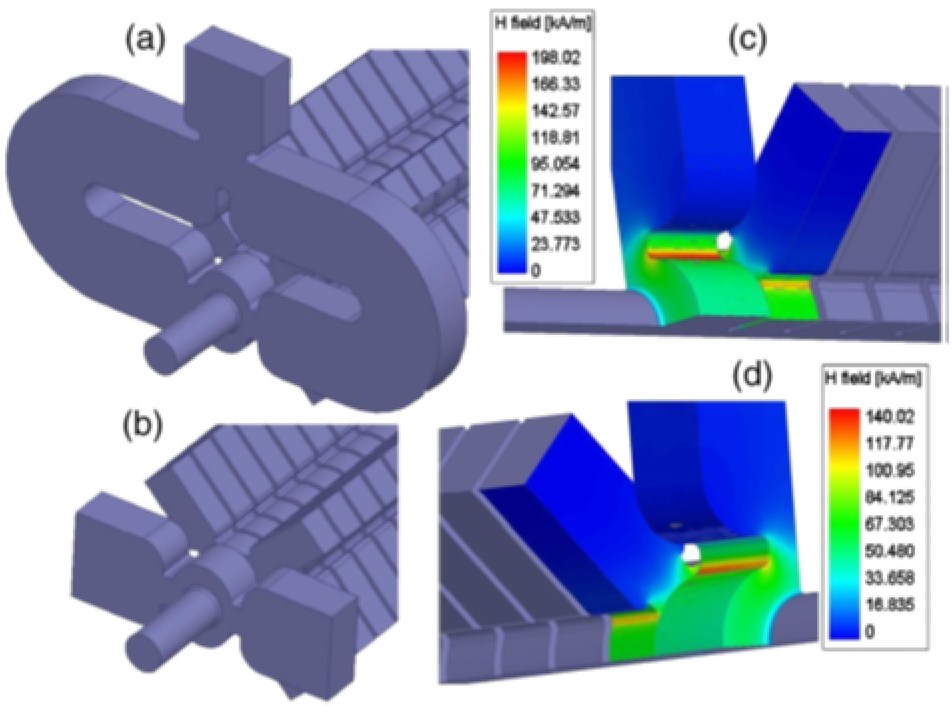


Figure 7: (a) input coupler; (b) output coupler; (c) surface magnetic field at the input coupler corresponding to $E_{acc}$ = 33 MV/m; (c) surface magnetic field at the output coupler corresponding to $E_{acc}$ = 33 MV/m

Once couplers are designed, the final step is to perform an electromagnetic simulation with HFSS of the whole structure (power couplers and cells). It allows to perform a fine tuning of cells and couplers checking the reflection coefficients and the on axis electric field flatness and to obtain a 3D field map that is useful for beam dynamics simulations. In Fig. 8, the longitudinal electric field profile along the whole structure simulated by HFSS is reported (ELI-NP).

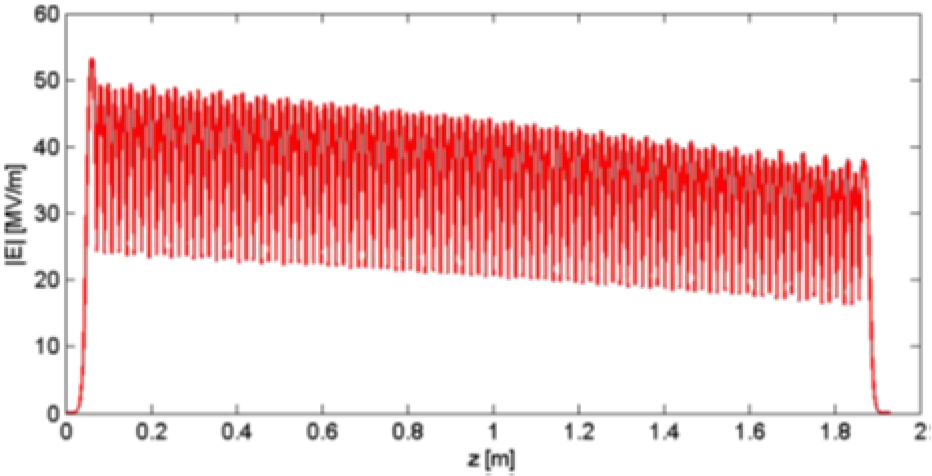


Figure 8: Longitudinal electric field profile along the whole structure simulated by HFSS

# 3 Project Breakdown Structure (PBS) for the linac

## 3.1 Introduction

A complete and well-structured documentation is a key tool to assess the progress of any project and to communicate to the project participants the outcomes of the development work. In the case of CompactLight, which aims at providing advanced conceptual design and manufacturing information to a wide community of potential user, the quality of the documentation is one of the main project goals and a major deliverable. Beyond the ultimate goal of building the project documentation, the availability of a shared space to store the reference documents and the specification tables would allow all project participants to base their design work on a common tool, immediately accessible, to exchange information at their latest release and to get very quickly an overview of the project advancement at any moment.

In the WP4, we have chosen to adopt the CERN Engineering Data Management System (EDMS) as the document repository, since it is a well-established, structured and regularly backed up data base. It supports document versioning and provides the possibility to apply an approval procedure to those documents that require it, for example if a quality assurance scheme needs to be introduced. It also allows to modulate the visibility of those documents that may have sensitive content, by making them accessible to a restricted group of readers that can be dynamically adapted to the project needs.

It is our intention to test this tool for the needs of WP4 first and we consider the possibility to propose an extension of this approach to the whole CompactLight project, if this first experience shows to be satisfactory.

## 3.2 The PBS

As a first step in the document organisation the tree structure of the project, in this case restricted to WP4, must be defined. Since the goal is to document the technical developments concerning the realisation of a FEL facility, based on X-band technology, the logical approach appears to be the adoption of the physical structure of the facility as a reference. This choice would help designers to follow the evolution of the development work in each area of the facility also by using the possibility to adopt incrementing versions of the study documentation. The sharing of up-to-date information in the form of parameter tables and design documents will help the daily work of development. In the particular case of WP4, being its responsibility focused on RF systems and the linac, we have chosen to split the linac components over three levels of progressively increasing detail, so to provide the necessary granularity.

In order to be consistent with a possible future extension of this approach to the CompactLight project, a preliminary structure has been sketched for the whole facility, without providing details. This will be further discussed within the project at a later stage and agreed among the persons in charge of the different workpackages.

Within this structure, the specification tables for each area of the machine will be the first kind of documents that should appear in each branch of the tree. Typical documents that should also be part of this documentation are Engineering functional specifications and interface specifications; both of which will help designers to always keep the problem of interfacing with nearby equipment and with the general infrastructure well into consideration. Prototype testing procedures and reports should also become part of this documentation, whenever applicable.

Fig. 9 shows the preliminary PBS proposed for the CompactLight facility.

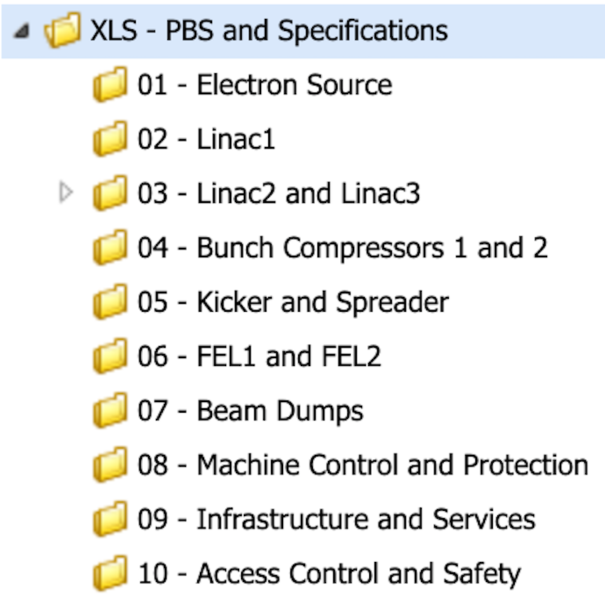


Figure 9: General PBS proposed for the CompactLight project

Fig. 10 shows the PBS that has been adopted by WP4 for the CompactLight linac.


Figure 10: Adopted PBS by WP4 for the description of the Main Linac in CompactLight

# 4 Gyroklystron, linearizer pulse compressor, and waveguide system: RF design and beam tracking tools

## 4.1 Introduction and requirements

The CompactLight X-FEL requires low emittance and a high energy electron beam to generate radiation. The off crest X-band acceleration and the higher order optics in the magnetic chicane will result in an energy slope nonlinearity. This nonlinearity may cause very sharp temporal spikes and longitudinal wakefields in the undulator section. A deceleration structure operating at the harmonic of the X-band (∼12 GHz) acceleration frequency can be used to compensate the energy nonlinearity. A third harmonic signal corresponding to a frequency of 36 GHz and a fourth harmonic signal corresponding to a frequency of 48 GHz to be used to drive a lineariser have been chosen and are currently being investigated. The higher the harmonic, the less amplitude (and thus RF power) required but this needs to be balanced by the increased difficulty in producing high power radiation as the frequency increases. However operating at a higher harmonic also helps to reduce the length of the lineariser.

The lineariser is to be driven by MW level high power microwave radiation at 36 GHz or 48 GHz using gyrotron klystron amplifiers but as yet such amplifiers are not commercially available. The Strathclyde team is responsible for designing a gyrotron klystron amplifier operating at 36 GHz or 48 GHz with peak output power of up to 3.0 MW and 1.5 MW, respectively. A three-cavity Ka-band MW-level gyroklystron operating at the fundamental $TE_{02}$ mode in the output cavity while the input and bunching cavities are operating with the $TE_{01}$ mode has been designed. The initial parameters of the electron beam were established by the linear and nonlinear theory of the electron cyclotron maser instability. The geometry parameters of the interaction circuit were established by the field-matching theory and a scattering matrix method, and further accurately simulated by the electromagnetic solver to validate the cavity performance. A loss load structure was employed to adjust the $Q$ factors of the gyroklystron cavities and to apply RF loss in the drift tunnel, to match the gyroklystron requirements. The structure of the interaction circuit was matched to the uniform field region of the magnet. As a trade of the performance of the interaction efficiency, gain and bandwidth, a three-cavity design for the gyroklystron, as shown in Fig. 11 was chosen. (1) is the input cavity, (2) is the 1$^{st}$ drift tunnel, (3) is the bunching cavity, (4) is the 2$^{nd}$ drift tunnel, (5) is the output cavity and (6) is the collector.

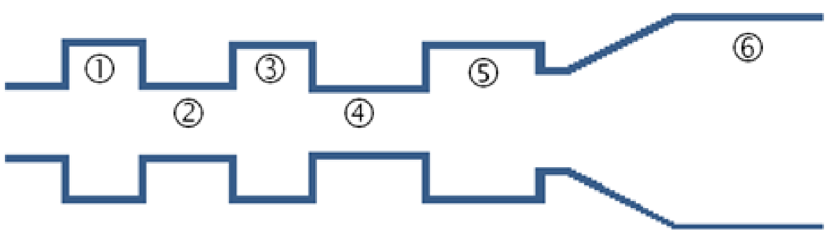


Figure 11: The schematic diagram of the three-cavity gyroklystron

The interaction structure was optimised using the Particle-In-Cell code MAGIC to obtain an output power of 1.9 MW, as shown in Fig. 12. An interaction efficiency of 44% was achieved in the simulation with an electron beam of voltage 95 kV and current 45 A.

The Fourier transformation of the amplitude of the electric field at the output port is shown in Fig. 13. A distinct frequency component of 36 GHz exists in the frequency spectrum. No other frequency components were found except a relatively weak 2nd harmonic frequency component at 72 GHz and a 3rd harmonic frequency component at 108 GHz.

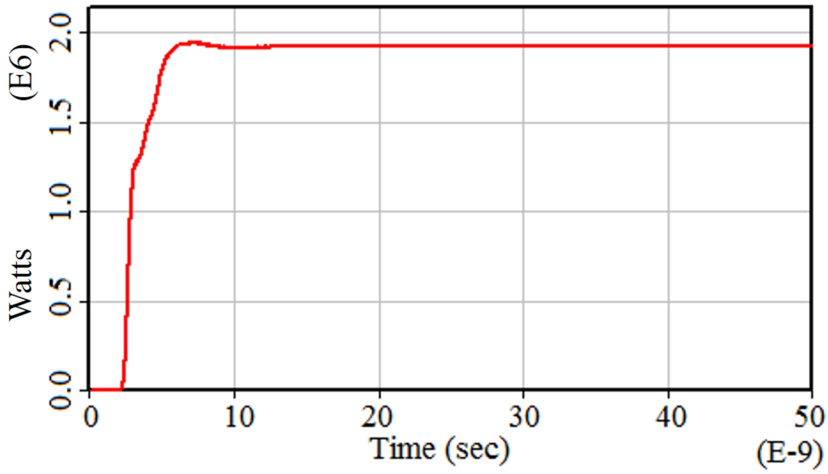


Figure 12: Ouput power as a function of the time

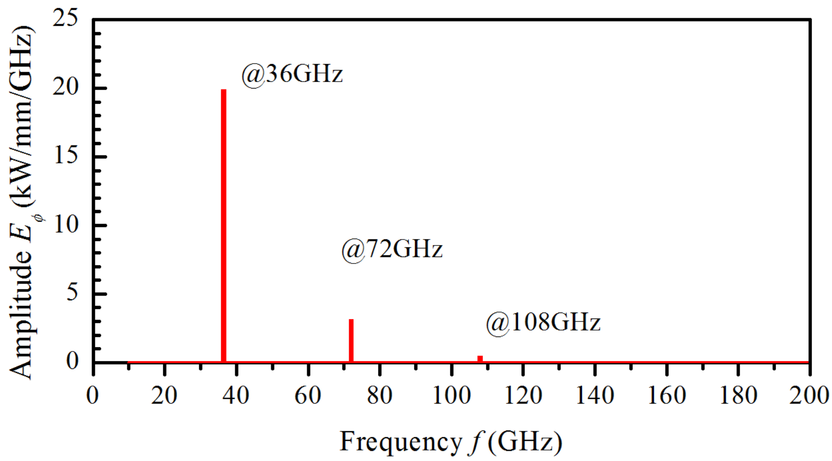


Figure 13: The schematic diagram of the three-cavity gyroklystron

The lineariser is to be driven by MW level high power microwave radiation at 36 or 48 GHz using gyrotron klystron amplifiers but as yet such amplifiers are not commercially available. The Strathclyde team is responsible for designing a gyrotron klystron amplifier operating at 36 or 48 GHz with a peak output power of 3.0 and 1.5 MW, respectively. A pulse compressor with a compression ratio of 4 is also being developed by colleagues at CERN. A combination of the gyrotron klystron amplifier and the pulse compressor will be used to drive the lineariser to be developed by colleagues at the University of Lancaster.

## 4.2 Linearizer pulse compressor and waveguide system

### 4.2.1 Introduction

The gyrotron klystron designed by Strathclyde team is the power source for the Ka-band lineariser structure developed by the University of Lancaster from WP3. From initial studies, required peak powers are in the range of 3.0 MW and 1.5 MW at 36 GHz and 48 GHz respectively [9]. However, this output power is likely not sufficient to reach the desirable gains in the lineariser based on the beam dynamics calculation from WP6 [10]. Therefore a pulse compressor and related power transfer system are required and are part of the baseline design. A power gain of four times can be achieved by the pulse compressor, e.g., SLEDII type pulse compressor [11]. It gives a comfortable margin for the operation of the lineariser. As normal rectangular waveguide at 36 GHz or 48 GHz has a high loss, the overmoded waveguide component will be a good solution for the low loss power transfer system [12–15]. These RF systems require further dedicated simulation tools, and these are described below.

#### 4.2.2 Design process

1. Set the RF parameters (Q factor, shunt impedance, and group velocity) and length of the Ka-band lineariser (input from WP3).
2. Set the linearising voltage (input from WP6) and define the input for the lineariser.
3. Set the power gain of the Ka-band pulse compressor based on the output of the gyrotron klystron
4. Electromagnetic design and optimization of the pulse compressor and the related power transfer system.
5. Finalise the electromagnetic design: input and output couplers.

Iterations cycles are required based on the discussions and data exchange with other WPs.

#### 4.2.3 Software tools

Similar to the RF system design introduced in § 2.3, three commercial computer codes, HFSS, CST Microwave Studio, and MATLAB, are used in the design and optimization. The electromagnetic field and the RF parameters such as Q factor, and modified Poynting vector of the pulse compressor can be calculated by HFSS and crossed checked with CST Microwave Studio.

### 4.3 Gyrotron klystron

The gyrotron klystron is a vacuum electronic based amplifier that relies on the fast beam-wave electron cyclotron maser interaction for its operation. Compared with a conventional klystron normally used in the accelerators, the gyrotron klystron has the advantages of being able to achieve MWs of power at high (Ka-band) frequency. The main components in a gyroklystron include: the Magnetic Injection gun (MIG) to generate a rotating electron beam with optimised transverse to axial velocity ratio and small velocity spread; beam-wave interaction circuit to effectively convert the power in the electron beam into the microwave radiation; a cryogen free superconducting magnet system to properly guide the electron beam and maintain the electron beam cyclotron frequency; the coupling system to couple the input and output radiation; the ultra-high vacuum system; and the energy recovery system to reduce the thermal load when operating at high pulse repetition frequencies of 1 kHz.

### 4.3.1 Design process of the gyroklystron

The general design process of the gyroklystron includes:

1. The estimation of the operating parameters of the gyroklystron based on the cyclotron maser instability, including the operating cavity mode, electron beam voltage, beam current, magnetic field strength and the beam transverse to axial velocity ratio.

2. Determination of the interaction circuit structure based on the small signal linear theory, including the number of cavities and the parameter range of the cavity dimensions.

3. Detailed calculation of the gain, bandwidth that can be achieved from the optimised parameter range based on a nonlinear large signal simulation.

4. Accurate simulation of the beam-wave interaction based on Finite-difference Time-domain Particle-in-Cell simulation of the optimal geometry suggested by the nonlinear theory calculations. This enables the space charge effect in the gyroklystron cavities, the beam energy spread, velocity spread to be included in the simulations. The design goal is to achieve the required output power, frequency and efficiency from a gyrotron klystron amplifier that can be manufactured with acceptable tolerances.

5. Design the MIG gun based on the simulation and optimisation of the interaction circuit. Synthesis of the electron gun geometry based on the conservation of the angular momentum following by a global optimisation routine.

6. Configuration of the superconducting magnet design to match the requirement for the MIG gun.

7. Microwave components, including the input coupler, output mode converter, and high power microwave windows.

8. The thermal load calculations in the waveguide structures, interaction region as well as the collector region. Adjustments of electron beam parameters to ensure the thermal load is kept under within a safe operating region while operating at high pulse repetition frequencies of 1 kHz.

### 4.3.2 Required simulation tools

The simulation tools required to complete the simulation of a gyrotron klystron amplifier includes:

1. A small signal linear and large signal nonlinear code developed in house to quickly predict the performance of a gyroklystron.
2. 2D/3D Finite-difference Time-domain Particle-in-Cell simulation software (for example MAGIC) used to simulate the interaction efficiency of the gyrotron klystron.
3. SIMULIA (CST Particle Studio). The 3D particle tracking tools used to calculate the magnetic field from the superconducting magnet, as well as the beam trajectories of the MIG gun.
4. SIMULIA (CST Microwave Studio) used to calculate the Eigenfrequency of the designed cavity of the gyrotron klystron, as well as simulate the scattering parameters of the microwave windows, mode converters and input/output couplers.
5. ANSYS used to simulate the thermal load inside the cavity as well as the collector region.
6. In house developed optimization platform based on a multiple-objective optimization platform programmed in C++ to be used to enhance the simulations being conducted to optimise the parameter sets to achieve the design goals.

# 5 Conclusion

All of the essential design tools for the CompactLight linac have been established and have even been used to establish preliminary designs for most critical hardware elements. In addition, exchanges of critical parameters from other work packages and/or corresponding parts of the facility have been made. This puts WP4 in a position to establish and document baseline designs of the critical hardware elements on schedule.

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