ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-WEPR73

# C-BAND HIGH-GRADIENT LINAC DESIGN CONSIDERATIONS FOR HPC MODELING

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*Abstract*

The production of soft to hard x-rays (up to 25 keV) at XFEL (x-ray free-electron laser) facilities has enabled new developments in a broad range of disciplines. However, there is great potential for new scientific discovery at even higher energies (42+ keV). For next-generation state-of-art facilities such as DMMSC (Dynamic Mesoscale Material Science Capability) at Los Alamos National Laboratory, C-band technology shows great potential. In general, these research instruments can require a large amount of real estate, which quickly can escalate costs and limit the location of the device. It has been shown in recent work that linacs designed for use in the C-band frequency range (c.a. 5712 MHz) are well-suited for these FEL's due to their size and performance.

There are multiple geometrical considerations that contribute to a cavity's performance, such as cavity shape, size, material, etc. There are often many aspects that interplay to create a customized structure with suitable figures of merit and hence performance. Simulations help illustrate the point. Here, we describe a possible scheme for preparing an elliptical geometry for parameter variation at the ALCF.

The Argonne Leadership Computing Facility (ALCF), located at Argonne National Laboratory, is a key tool to facilitate our investigations of design concepts [1]. The combination of access to a HPC facility such as the ALCF and software that can run at this facility are an effective combination. We have access to the ALCF through the ALCF LIGHTCONTROL project.

We used VSim 12.0.3 to investigate different geometries for accelerator applications at a C-band frequency [2]. It is designed for HPC environments and is already in use at the ALCF.

## INTRODUCTION

X-ray Free Electron Lasers (XFEL) are driven by a high energy electron linear accelerator, where the need for higher energy X-rays requires higher electron beam energies. To first order, this requires longer LINACs and larger infrastructure, which quickly makes the costs prohibitive. Next generation XFELs, such as FEL projects planned at LANL [3] and UCLA [4,5], will take advantage of high-gradient, compact accelerating structures in the C and X-band frequency regimes, which will allow a better use of the available physical space. In C-band structures, cavity dimensions are on the order of a few centimeters, making them very compact as compared to cavities used in previous generation light sources. Design concepts have been discussed in [6] A state-of-art C-band linac with a 50 MV/m accelerating gradient requires approximately 200 m to produce a 10 GeV electron beam. This will be about 700 m long if using more traditional S-band technologies at around 15 MV/m [7].

In other words, C-band linacs are small enough to provide beams with suitable characteristics but not so small that they become extremely expensive to fabricate due to high tolerance requirements and other design considerations. C-band structures can generate higher electron beam energies capable of generating higher energy X-rays. Smaller structures, such as those designed to operate in the X-band also suffer from RF breakdown, which degrades performance over time. The reduced footprint is amenable to saving costs associated with real estate.

C-band design considerations must be incorporated into the actual design by using 3D EM simulations. As systems become more complex and structures require refinement, especially in a regime where particle beams must be optimized, or where material/beam interactions become important, increasing the amount of computing power is warranted to efficiently carry out simulations.

The number of variables that have to be considered during the optimization process can make desktop simulations intractable. We investigate some effects that small changes in geometry construction via a drawing program such as Autodesk Fusion 360® for personal use on an elliptical traveling wave (TW) structure modelled for operation at f =5.712 GHz.

## EM MODELING OF ACCELERATING STRUCTURES

C-band structures are high-frequency structures and do not generally have an analytical solution, requiring simulation codes. There are a host of options, but it is necessary in this case that a software package suitable for HPC environments be adopted. VSim fits this requirement and has well-developed particle-in-cell (PIC) capabilities. VSim is based on the Vorpal engine [8] and is well suited for electromagnetic and charged particle problems like the ones involved in cavity design. We use Vsim for EM simulations.

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15th International Particle Accelerator Conference,Nashville, TN JACoW Publishing
ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-WEPR73

Vsim works in 1, 2, or 3 dimensions, facilitating EM simulations using algorithms designed for high performance computing and is already in use at the ALCF.

Elliptical cavities are subtle to construct. They consist of two elliptical arcs connected by a straight line as shown in Fig. 1. There are seven independent variables that govern this construction, and some of them are predetermined when selecing the frequency range of interest. Table 1 describes these parameters. The structure has a cell length equal to λ/3 to match the phase velocity of the travelling electromagnetic wave to the velocity of relativistic electrons. This corresponds to a 2π/3 phase advance between adjacent cells. VSim has an example simulation that uses an algorithm that can be used to generate an elliptical geometry and calculate eigenmodes [9,10]. An elliptical C-band accelerating structure is shown in Fig. 2.

This example can be used as a "building block" of a more

complex construction, such as a C-band waveguide with a waveguide coupler assembly. The text-based example allows one to set values of the frequency band, the number of cells, the cavity radius Rmax, and the curvature radii, ρmin and ρmax. The parameter ZSQUASH, can be 0 for a cavity array with cylindrical symmetry, or can be set to a value such as 0.0025 to squeeze the cells to suppress degeneracy due to cylindrical symmetry. Running this simulation to tune it to 5.712 GHz with a 2π/3 phase advance can take many iterations.

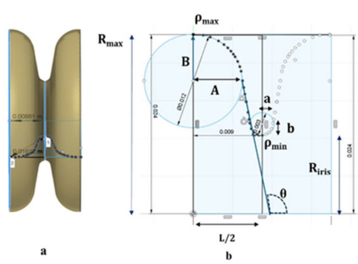


Figure 1: An elliptical cavity cell (a), and (b) a sketch used to generate the cell parameters from Table 1.

Table 1: Selected C-band Design Parameters

| **Parameter** | **Description** |
|---|---|
| $R_{max}$ | Frequency tuning |
| $R_{iris}$ | Cell coupling |
| $\rho_{max}$ | Radius of curvature cell |
| $\rho_{min}$ | Radius of curvature iris |
| ½ Cell Length, L/2 | βλ/3; β=v/c~1 for e's |
| A, B, a, b, θ | 4 of 5 are independent; choose 4 |

Geometries in Vorpal are non-grid-aligned material shapes. They can be defined in several ways, e.g., a triangular surface mesh from an STL file, a set of shapes from a STEP file, Constructive Solid Geometry (CSG), and functional, which is a function defining whether a point in space is inside or outside. One can import both. stl and Python-defined shapes. CAD geometries can also be used in conjunction with CSG primitives built in VSim.

The time step is also important. An additional relation denoted DMFRAC incorporates the Courant Condition (cfl) and the Dey-Mittra Fraction (DMfrac). [11] The Dey-Mittra algorithm allows for 3D modeling of complex curved surfaces with less computational demand than Finite-Difference methods. It is used to control the stability of the simulation and gives 2nd order solution accuracy. It ranges from 0 to 1 and is related to the Courant Condition as a multiplicative factor for solving partial differential equations [12].

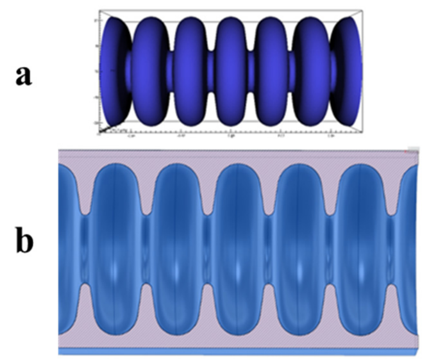


Figure 2: The elliptical geometry as generated by the Vsim example simulation (a) and the geometry generated via a drawing program (b)

In this case, a customized structure was built by using VSim to generate an elliptical cavity array by using the example. Here, an elliptical structure was created in a drawing program based on a VSim macro-created geometry. This array was imported into Fusion 360 and converted into a cavity in a block of material. A waveguide coupler was constructed, and coupler aperture was created in the blocked cavity array. These components were assembled in Fusion and imported into VSim as an STL file. The components could alternately be imported into VSim separately and aligned there. Initial EM analysis was done in a desktop setting.

For a C-band excitation, the waveguide launcher used was equivalent to a WR-159, with a frequency band of 4.90 to 7.05 GHz, a lowest order mode cutoff frequency of .712 GHz, and dimensions of 1.59 Inches [40.386 mm] x 0.795 Inches [20.193 mm]. See Fig. 3. Fig. 4 Shows the eigenmode pattern for a resonant frequency of 5.712 GHz. It is possible to run scripts on POLARIS for the purpose of parameter variation and will be employed in the future for linac optimization.

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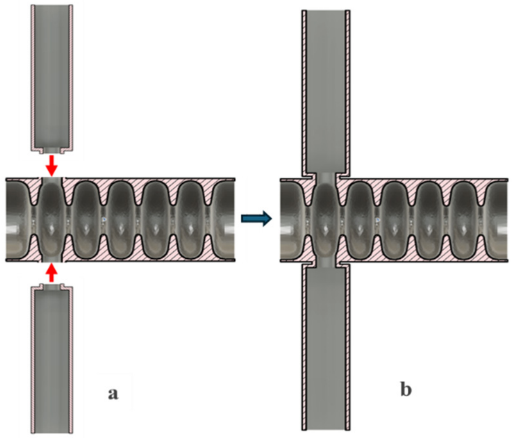


Figure 3. The a) modified elliptical structure and waveguide couplers as modular entities, and b) the finalized assembly after import into Vsim for simulation.

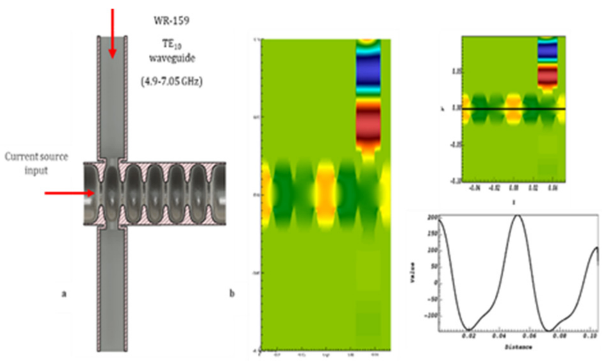


Figure 4. The modified elliptical structure with a waveguide coupler and (left) the array eigenmode pattern (right). The resonant frequency was $f$ = 5.712 GHz and phase advance 2π/3

## CONCLUSIONS

We are using Vsim to investigate different geometries for accelerator applications at a C-band frequency. For next generation XFEL technology. It should be noted that the procedure described here is not the only way to create a geometry that can be increasingly complex, owing to the many parameters that are inter-related. This does provide a more visual way to create geometries without creating code that can get increasingly complex. For example, it may be necessary to taper the inter-cavity irises or adjust the length of the end cavities. The curvature of the irises may have to be adjusted to mitigate RF breakdown. We provide a proof-of-principle result that demonstrates that we are moving towards advanced C-band geometry optimization at the ALCF. Also, as other characteristics are identified for optimization, *such as* additional fabrication challenges that need to be factored into the budget [13,14].

Finally, it must be stressed that this simulation program is compatible with HPC environments and has PIC capability. Particle simulations are a major factor in simulation time and file size, and running repeated simulations during parameter variation will become intractable.

## ACKNOWLEDGEMENTS

Many thanks to John Cary of Tech-X, for ongoing discussions. This work was performed under Contract No. 89233218CNA000001, supported by the U.S. Department of Energy's National Nuclear Security Administration, for the management and operation of Los Alamos National Laboratory (LANL). This research also used resources of the Argonne Leadership Computing Facility, a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357, and computing resources from Element Aero.

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