

# EIGENVALUE CALCULATIONS BASED ON THE FINITE ELEMENT METHOD WITH PHYSICALLY MOTIVATED FIELD SMOOTHING USING THE KIRCHHOFF INTEGRAL\*

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## Abstract

In current linear particle accelerators, the actual acceleration of the charged particles is realized with the help of the electric field strength within driven radio frequency resonators. The characterization and optimization of the applied resonating structures can be reliably performed on the basis of numerical simulation techniques. In the last decades, efficient numerical methods have been introduced to determine the electromagnetic fields in various structures.

Although the resonators are operated in a driven setup, one of the advantageous numerical strategies is given here by an eigendecomposition of the fields, which is realized by the application of accurate eigenmode calculations together with suitable post-processing steps. In particular, the extraction of representative field maps used for particle tracking requires an accurate numerical modeling of the fields at any position inside the structure. In order to avoid numerically motivated discontinuities of the fields, a proper smoothing algorithm based on the vector equivalents of the Kirchhoff integral is proposed.

## INTRODUCTION

The calculation of eigenfields in closed resonating structures belongs to one of the standard tasks within particle accelerator component design. In contrast to broadband field excitations where a huge number of contributing modes have to be considered, the classical eigenvalue calculation is preferably applied to narrow-band applications with a manageable number of modes. While the broadband case is profitably treated in the time domain, the effects of narrow-band excitations are advantageously processed with the help of proper eigenvalue solvers.

Because of the complex geometrical shapes of the incorporated accelerating cavities, a precise analytical treatment of the problem is impossible. An alternative is given by a numerical approach where the designated introduction of proper degrees of freedom enables to determine at least an approximate solution. The ultimately achievable accuracy of the numerically calculated eigensystem depends on the applied numerical method together with the provided number of degrees of freedom.

The continuity of all field components especially in the region where the charged particles are located naturally depends on the chosen discretization scheme. In particular, the

widespread finite element method (FEM) combined with Whitney-type basis functions show unphysical, discontinuous field components even in the vacuum part of the structure. If the field is further evaluated on an unstructured tetrahedral mesh, large axial field components can artificially couple to transverse components, which further emphasizes the need for a suppression of parasitic field components. This fundamental behavior can be observed also for various other numerical methods such that a proper smoothing of the fields is mandatory.

While generally any smoothing technique can be applied to the calculated fields, a physically motivated variant based on the Maxwell's equations is favorable. The aim of the smoothing is to reduce the numerically motivated discontinuity of the electromagnetic field components without introducing parasitic charges into the computational domain. Among the suitable methods, a vector equivalent of the Kirchhoff integral is proposed here because of its simple applicability. The smoothing effect is based here on the superposition of individual spherical waves, which originate from the freely selectable evaluation surface. A limited number of waves can be considered for the reconstruction of the electromagnetic fields if the required integration on the evaluation surface is carried out by numerical means using a finite number of collocation points.

## NUMERICAL MODELING

A favorable numerical description of the underlying electrodynamic eigenvalue problem is based on the Maxwell's equations in frequency domain

$$\text{curl } \vec{H} = \vec{J} + j\omega\vec{D} \quad (1a)$$

$$\text{curl } \vec{E} = -j\omega\vec{B} \quad (1b)$$

$$\text{div } \vec{B} = 0 \quad (1c)$$

$$\text{div } \vec{D} = \rho \quad (1d)$$

where the symbols  $\vec{E}$  and  $\vec{H}$  are used to represent the electric and magnetic field strength. On account of the aimed application, the corresponding electric and magnetic flux density can be related to the electromagnetic field according to linear, isotropic material relations which results in the simple description  $\vec{D} = \epsilon_0\epsilon_r\vec{E}$  and  $\vec{B} = \mu_0\mu_r\vec{H}$ . The necessary sources are described by the electric charge density  $\rho$  together with the electric current density  $\vec{J}$  while  $\omega$  is used to represent the angular frequency.

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In the following, we eliminate the dependency on the magnetic field and concentrate on a description of the electric field only which allows to approximate the field distribution by

$$\vec{E}(\vec{r}) = \sum_{i=1}^N x_i \vec{\omega}_i(\vec{r}), \quad \vec{r} \in \Omega. \quad (2)$$

Usage of a tangentially continuous set of weighted Nédélec-type basis functions  $\vec{\omega}_i(\vec{r})$  enables to evaluate the electromagnetic field in the entire computational domain  $\Omega$ . Once the weighting coefficients  $x_i$  are collected in the complex-valued vector  $x = (x_1, \dots, x_N)$ , the generalized nonlinear eigenvalue problem

$$A(\omega) x = \omega^2 \mu_0 \epsilon_0 B x \quad (3)$$

is derived on an algebraic level employing Eq. (1) and Eq. (2) while no sources have to be considered explicitly. According to the weighted residual procedure of the applied FEM, the contributions to the stiffness matrix  $A$  as well as to the mass matrix  $B$  are given in terms of integrals over the entire computational domain  $\Omega$

$$A_{ij} = \iiint_{\Omega} \frac{1}{\mu_r} \text{curl } \vec{\omega}_i \cdot \text{curl } \vec{\omega}_j \, d\Omega + \text{losses} \quad (4a)$$

$$B_{ij} = \iiint_{\Omega} \epsilon_r \vec{\omega}_i \cdot \vec{\omega}_j \, d\Omega \quad (4b)$$

with element-wise defined basis functions. To simplify the computation, the matrices are assembled with respect to the discretized volume only such that the integration can merely concentrate on individual grid elements.

All possible loss mechanisms like surface losses or port contributions are represented in the stiffness matrix to leave the mass matrix untouched, such that the fundamental property of a positive definite matrix  $B$  will be retained even in the lossy case [1]. As a result, the stiffness matrix  $A$  will depend on the frequency and a nonlinear problem emerge. Solving the eigenvalue system specified in Eq. (3) enables to evaluate the approximation given in Eq. (2) at any position inside the computational domain  $\Omega$ .

### Kirchhoff Integral

For some particular applications, the numerical evaluation of the electromagnetic field components within the computational domain leads to an unwanted behavior. This phenomenon can be particularly observed in a case, when the sampling of the field is so high that multiple evaluation points are located within a single computational element. Moreover, the same situation takes place even for a coarse sampling where field evaluation points are assigned to distinct computational elements. Here, an undesired numerically motivated coupling of strong field components from one direction to the others can superimpose to real physical fields such that small field variations may be lost. In such cases, a smoothing of the extracted field components is advantageous to damp the undesired field variations to an acceptable level.

One of the critical applications is given for example in the area of accelerating radio frequency cavities where a precise knowledge of the electromagnetic field is required for both component characterization and beam dynamics studies. In contrast to a multitude of smoothing algorithms where the remaining field does not satisfy the Maxwell equations in a specified domain, the application of physically motivated variants can bypass this difficulty.

Among the promising techniques is the vector equivalent of the Kirchhoff integral [2], which uses a large number of spherical waves to represent the electromagnetic field inside a given domain from the known equivalent values on the corresponding closed surface. The evaluation area can be chosen arbitrarily so that even a subset of the enveloping surface of the computational domain can be considered. This procedure with reduced efforts is profitable in case when field evaluation points are limited to a given region where the enveloping surface can be simplified significantly. This is in particular the case, when field values near to the cavity axis have to be extracted, as it is often the case for beam dynamics studies.

The vector equivalents of the Kirchhoff integral can be formulated for the electric field strength as well as for the magnetic flux density. Both fields are required for subsequent particle dynamics investigations. In order to simplify the notation, the profitable substitution  $\vec{B}' = jc\vec{B}$  will be used with  $c$  representing the speed of light in the homogeneous subregion. This notation enables to formulate the integrals

$$\vec{E} = \iint_A \left( (\vec{n} \times \vec{B}') k G - (\vec{n} \times \vec{E}) \times \nabla G - (\vec{n} \cdot \vec{E}) \nabla G \right) dA \quad (5a)$$

$$\vec{B}' = \iint_A \left( (\vec{n} \times \vec{E}) k G - (\vec{n} \times \vec{B}') \times \nabla G - (\vec{n} \cdot \vec{B}') \nabla G \right) dA \quad (5b)$$

in a symmetric way using  $\vec{n}$  as the unit normal directed *out* of the enclosed volume and  $k = \frac{\omega}{c}$  to represent the propagation constant. Special care has to be put on a proper evaluation of the individual components because deviating definitions especially of the direction of the unit normal but also of the sign of the angular frequency in various publications lead to deviating results. The important contribution is originating from the Green's function

$$G = \frac{e^{-jkr}}{4\pi r}, \quad r = |\vec{r}_P - \vec{r}_Q| \quad (6)$$

where the observation point  $\vec{r}_P \in \Omega$  is located inside the computational domain and the source point  $\vec{r}_Q \in A$  lies on the chosen evaluation surface. According to Eq. (5), the tangential as well as the normal component of the electric field strength and the magnetic flux density are simultaneously required. We do not explicitly eliminate the mutual dependency as it is performed within the boundary element method for example but evaluate all necessary field components from the known FEM solution in a post-processing step. The ultimate smoothing is therefore automatically obtained with the help of the stated Kirchhoff integrals.

## APPLICATION

A proper design of radio frequency accelerating cavities requires the precise knowledge of the predominant electromagnetic fields inside a given structure. This information is necessary for both beam dynamics and for characterization of the investigated component itself. Concentrating on the fundamental accelerating mode, any extraction of a corresponding field can be obtained with the help of a suitable numerical method, where an eigenmode calculation based on the FEM is well established.

In the following, a TESLA 3.9 GHz cavity [3] will be examined as an illustrative classic example where special focus is put on the correct modeling of the coaxial high-power input coupler as well as the two attached higher-order mode couplers (Fig.1).

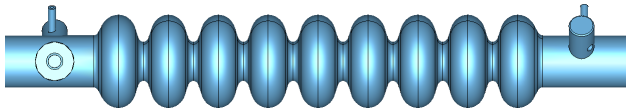


Figure 1: Computational model of a 9-cell third-harmonic TESLA 3.9 GHz cavity including the coaxial high-power input coupler as well as two higher-order mode couplers.

The actual cavity is built of high-purity niobium, which reaches a superconducting state when cooled using liquid helium. This condition allows to simplify the computational model drastically because even the simple perfect electric boundary condition can be applied without introducing too much errors. Due to the attached couplers, only the coaxial lines have to be modeled with the expensive port boundary conditions. This procedure enables to correctly model the intended energy extraction from the cavity, which naturally influences the field distribution inside the structure and has to be treated therefore with special care.

The FEM has been implemented with second order field approximation on curved tetrahedral elements whereas the CST Studio Suite [4] provides the required high-quality mesh. The implementation is based on PETSc [5] with an in-house realization of the Jacobi-Davidson eigenvalue solver to enable an efficient solution of the underlying nonlinear eigenvalue problem.

Once the desired eigenpair is found, the corresponding electromagnetic field distribution can be evaluated with the help of the approximation shown in Eq. (2) together with Faraday's law specified in Eq. (1b). The direct evaluation of the FEM data for a mesh consisting of 4 464 452 curved tetrahedral elements is shown in Figs. 2 and 3 in gray and black color. Unphysical oscillations especially inside the cavity region can be observed which are unsuited for further processing steps.

A physically motivated smoothing process is given with the vector equivalents of the Kirchhoff integral specified in Eq. (5). A straightforward application of the given relations evaluated on a cylindrical envelope surface inside the specified cavity enables to provide smooth data, which can be immediately used for further analysis. For the specified application the obtained field components are displayed in

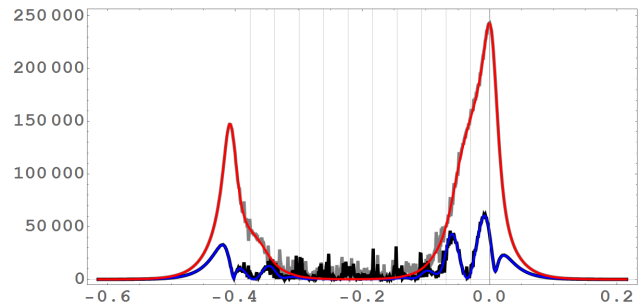


Figure 2: Smoothed (unsmoothed in gray/black) distribution of the electric field component  $E_x$  (red) together with the scaled magnetic flux density  $cB_y$  (blue) in V/m as a function of the longitudinal position  $z$  in m along the cavity axis.

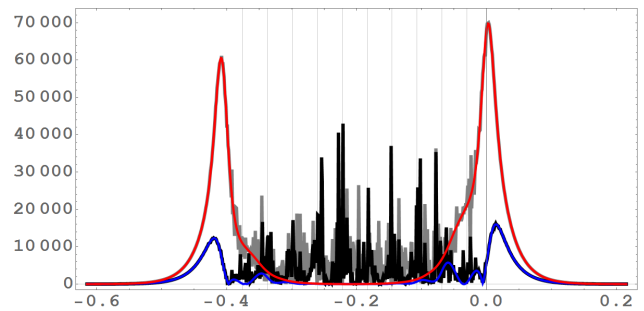


Figure 3: Smoothed (unsmoothed in gray/black) distribution of the electric field component  $E_y$  (red) together with the scaled magnetic flux density  $cB_x$  (blue) in V/m as a function of the longitudinal position  $z$  in m along the cavity axis.

Figs. 2 and 3 to support a direct comparison to the original FEM data. A clear improvement of the quality of the extracted electromagnetic field components is visible.

## CONCLUSION

The vector equivalents of the Kirchhoff integral are suited to smooth the electromagnetic field components of native FEM data on a physical basis with the help of individual spherical waves. The field continuity is sustained in domains with homogeneous material distributions independent on the original mesh-cell distribution.

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