IMPLEMENTATIONAL ASPECTS OF EIGENMODE COMPUTATION BASED ON PERTURBATION THEORY*

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Abstract

Geometry perturbations affect the eigenmodes of a resonant cavity and thereby can improve but also impair the performance characteristics of the cavity. To investigate the effects of both, intentional and inevitable geometry variations parameter studies are to be undertaken. Using common eigenmode solvers involves to perform a full eigenmode computation for each variation step, even if the geometry is only slightly altered. Therefore, such investigations tend to be computationally extensive and inefficient. Yet, the computational effort for parameter studies may be significantly reduced by using perturbative computation methods. Knowing a set of initial eigenmodes of the unperturbed geometry these allow for the expansion of the eigenmodes of the perturbed geometry in terms of the unperturbed modes. In this paper, we study the complexity of a numerical implementation of perturbative methods. An essential aspect is the computation and analysis of the unperturbed modes since the number and order of these modes determine the accuracy of the results.

INTRODUCTION

Aiming to design a cavity with best possible performance it is necessary to optimize miscellaneous of its characteristics that all depend on the cavity's eigenmodes. The cavity shape mainly influences these characteristics and has to be changed numerous times during the optimization process. Any geometry modification entails a full recomputation of the eigenmodes causing an immense total computational effort. Perturbative methods allow for avoiding this repetitive procedure. The methods (discussed here) base on the approach of computing the eigenmodes (denoted as unperturbed) of exclusively one initial geometry using a common computation method and deriving the eigenmodes (denoted as perturbed) of a modified geometry directly from the unperturbed eigenmodes with substantially less effort.

To do so, the interaction of each unperturbed mode i with every other unperturbed mode k has to be determined by forming an expression that includes their resonant frequencies f and a volume integration over the scalar product of their electric / magnetic fields $\mathbf{E}(\mathbf{r})$, $\mathbf{H}(\mathbf{r})$

$$\mathrm{IT}_{E(\mathrm{ik})} = \iiint_{\Delta V} \mathbf{E}_\mathrm{i}(\mathbf{r}) \cdot \mathbf{E}_\mathrm{k}(\mathbf{r}) \, \mathrm{d}V \qquad (1)$$

$$\mathrm{IT}_{H(\mathrm{ik})} = \iiint_{\Delta V} \mathbf{H}_\mathrm{i}(\mathbf{r}) \cdot \mathbf{H}_\mathrm{k}(\mathbf{r}) \, \mathrm{d}V \qquad (2)$$

Here ΔV is the volume that is removed by the modification from the unperturbed volume V. Applying further arithmetic operations to the resulting interaction term (IT) matrix finally yields the perturbed resonant frequencies and weighting factors that allow for expanding each perturbed electromagnetic field as a series of the unperturbed fields. In [1] and [2] two perturbative methods differing in the composition of their ITs and arithmetic operations are described in detail.

In [2] and [3] their applicability was proved by means of analytically evaluable cavity geometries providing very accurate results. Using analytically computed unperturbed eigenmodes all operations can be implemented with very high precision and very low effort. However, for most cavity structures the unperturbed modes have to be numerically computed. This is not only more complex and affected by additional numerical errors but also involves some difficulties that are discussed in the following. The numerical implementation was investigated using the example of a cylindrical cavity subject to one-dimensional perturbations to compare its outcomes with the analytically computed ones.

NUMERICAL IMPLEMENTATION

The computation of the unperturbed eigenmodes is the first and most expensive operation but has to be done only once for a certain cavity structure. It is required for the ITs and the series expansion and therefore particularly important for the accuracy of the results. The simulations are done with CST MWS Eigenmode Solver [4]. The integrals IT_E and IT_H solely depend on the fields in the boundary region (where the perturbation occurs). Besides an appropriate mesh density, hence a precise discretization of the boundary is significant. Since a discrepancy between discretized and actual boundary leads to an abrupt transition of the fields to zero (Fig. 1) an insufficient discretization may seriously impair the accuracy of the IT_E and IT_H. The Finite Element Method (FEM) combined with a tetrahedral mesh and curved elements proved to reproduce the boundary much more precisely than the hexahedral dual grid of the Finite Integration Theory (FIT). Therefore, here, FEM should be used for the eigenmode computation of cavities with a curved shape.

For the further processing the computed fields have to be exported from CST MWS as discrete field points. But despite the achieved precise boundary discretization using FEM some of these field values are still affected by the de-

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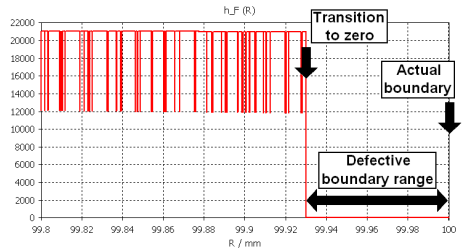

Figure 1: $\mathbf{H}_{\varphi}(r)$, cavity radius R: 100 mm, method: FIT. FEM-computed fields have a significantly smaller defective boundary range (0.3 μm) than the shown FIT-computed ones (70 μm) which are allocated on the dual grid in a certain distance to the boundary.

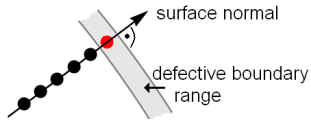

Figure 2: One-dimensional extrapolation of defective value (red) from correct values on the boundary surface normal.

fective boundary range. To minimize this impact a simple but effective procedure was developed. For it, each discrete field value that lies inside the defective region is extrapolated from a set of correct values located on the surface normal vector of the boundary (Fig. 2). By doing so, the accuracy of the ITs can be further improved.

For the computation of the ITs (done with Wolfram Mathematica [5]) two approaches were pursued. For the first approach, all discrete fields are interpolated to create continuous functions for the volume integration in Eqs. 1 and 2 in order to achieve a high accuracy. However, the computation of the interpolation functions and integrals turned out to cost an enormous effort. The main reason is that very accurate results can only be obtained by an interpolation of higher degree. But this can only be done on a structured grid which requires to interpolate the fields inside a larger volume than ΔV (in many cases the complete volume V) while the grid density must be kept appropriate for ΔV. Such a three-dimensional higher degree interpolation for a huge number of grid points is very inefficient. Consequently, an alternative approach was needed. Its main idea is to partition the volume ΔV into elements, determine the discrete field values in their centers and then substitute the integration by a summation of the products

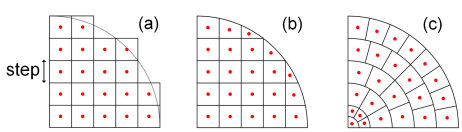

Figure 3: Volume partitioning of a cylinder (cross cut): (a) Pure cubic elements. (b) Cubic / (c) cylindrical elements with analytically determined boundary elements.

of the discrete integrands and volumes. These basic operations need only little effort and solely the fields inside ΔV have to be processed. But the commonly used partitioning into cubic elements (Fig. 3(a)) is not adequate for a summation over ΔV because of the required precise boundary discretization. Therefore, an improved partitioning algorithm was developed. If the boundary of ΔV and an element intersect volume and center of the element change. But both can be analytically computed due to the fact that usually all cavity shapes are described by (piecewise) analytical functions (Fig. 3(b),(c)). Correcting these intersection elements can essentially improve the accuracy of the IT_E and IT_H.

After the computation of all ITs, the arithmetic operations of the respective method (mostly matrix operations) have to be performed. These finally yield the perturbed resonant frequencies and the weighting factors of the series expansion. The operations are equal for analytically and numerically computed ITs and easy to implement with a low effort and very high accuracy. In case that besides the frequencies also the perturbed fields or certain cavity characteristics (e.g. E_{peak}/E_{acc} or Q_{ext}) are desired the complete or at least parts of unperturbed fields have to be previously exported to do the series expansion.

RESULTS

In the following, the implementational outcomes for a radial perturbation of a cylindrical cavity (R=100 mm, L=100 mm, fundamental mode of 1.15 GHz) investigating $\mathrm{TM}_{2.n.2}$ modes (n: radial mode index) are exemplarily discussed. The frequencies of the numerically computed unperturbed mode are highly accurate. The relative deviation is less than $1.6 \cdot 10^{-4}$ inside a very large frequency range (up to 35.71 GHz). Thereby an essential condition for the following operations is fulfilled since all intermediate and final results highly depend on the computable frequency range. However, it has to be considered that the accuracy degrades with increasing frequency due to the fact that the number of simulated mesh cells is limited by the available memory (Fig. 4).

To obtain accurate IT_E and IT_H the discrete volume elements have to be chosen small enough to properly discretize the fields of all unperturbed modes. While the IT_E and IT_H of modes with a low frequency can be computed

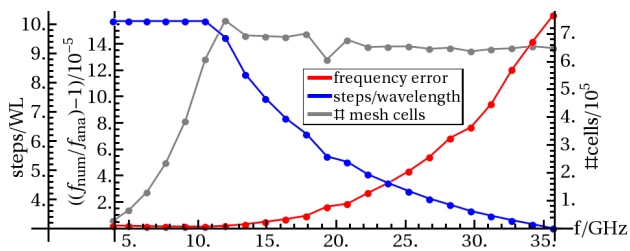

Figure 4: Parameters of CST MWS eigenmode computation of $\mathrm{TM}_{2.1.2}$ to $\mathrm{TM}_{2.23.2}$. The intended steps per wavelength reduce from 12 GHz on due to full memory usage.

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with very coarse elements their accuracy for higher modes largely depends on the element step size (Fig. 5(a)). However, a large perturbation does not require elements as fine as a small perturbation does (Fig. 5(b)). A very precise step size is only needed if the perturbation is also very small. Considering this, the efficiency can be increased by avoiding the use of an unnecessarily large number of elements.

Choosing volume elements with an appropriate discretization and effort, the relative deviation of the integral IT_E of the electrical fields is largely below $2 \cdot 10^{-3}$ and hence very accurate (Fig. 6). Only for comparatively small IT_E it rises up to $7.42 \cdot 10^{-3}$. The deviation of the IT_H is equal up to the 13th mode. The IT_H of higher modes are relatively small so that they are increasingly impaired by the numerical simulation error. As a consequence the relative deviation rises up to $3 \cdot 10^{-2}$. The accuracy of the final ITs depends on the used perturbative method. For [2] solely the IT_E are required so that the so computed ITs remain as accurate as the IT_E. But for the ITs in [1] the integrals IT_E and IT_H are multiplied by the further quantities and subtracted from each other. Thereby the relaitve error contribution of IT_E and IT_H changes. This may increase the deviation for some of the resulting ITs. Due to the complexity of the mathematical relations the details are not discussed here.

Compairing the final results, the perturbed frequencies $\tilde{f}$

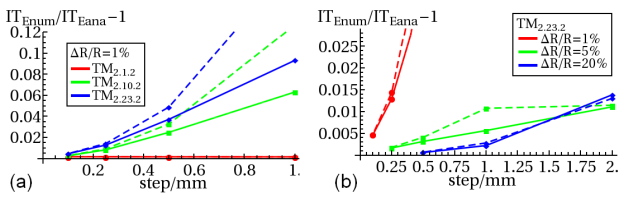

Figure 5: Relative error of selected $\mathrm{IT}_{E(\mathrm{ii})}$ depending on the step size of the volume elements (— cubic, - - - cylindrical) for different modes (a) and radial perturbations (b).

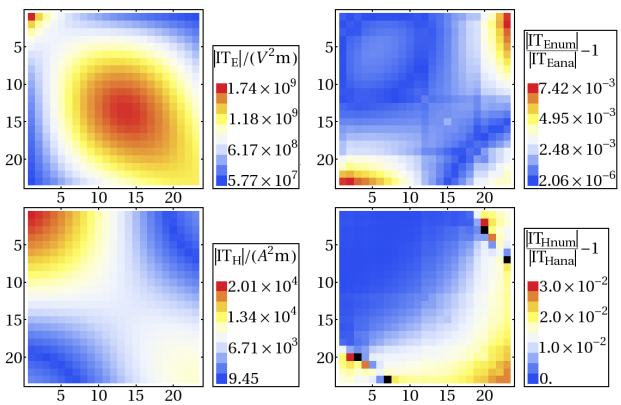

Figure 6: Absolute values and relative error of the IT_E and IT_H for radial perturbation of 5% using $3.4 \cdot 10^5$ cubic volume elements with 0.5 mm step size. For two IT_H that are almost zero the error is not shown (black areas).

based on a numerically implementation highly coincide with the ones based on an analytically implementation (Fig. 7). This proves the practicability and accuracy of a numerical implementation. Figure 7 also shows that the results using [1] deviate more from the expected ones than the results using [2] due to the previous described different composition of the ITs.

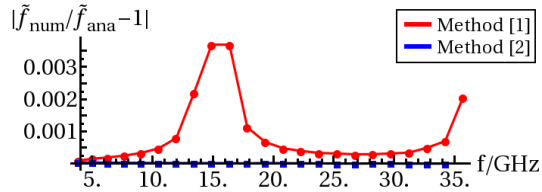

Figure 7: Relative deviation between perturbed frequencies based on numerically computed unperturbed eigenmodes and the ones based on analytically computed eigenmodes.

CONCLUSIONS

The investigations showed that a completely numerical implementation of perturbative methods using standard software is feasible. The development of special procedures for the processing of numerically computed unperturbed eigenmodes allows for a very accurate and efficient computation of the necessary basic parameters (unperturbed frequencies and volume integrals of the electromagnetic fields) over a large frequency range. The perturbed eigenmodes determined from these basic parameters very exactly match the results of analytically comparative calculations. But it also became apparent that there are differences in the error propagation depending on the algorithm of the used method which should be further examined.

The most important conclusion of the investigations is that the implementation algorithm described in this paper allows for the application of perturbative methods to any desired cavity geometry providing reasonable results.

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