Uncertainty Quantification for Complex RF-structures Using the State-space Concatenation Approach

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Abstract— In various applications of computational engineering and accelerator physics, the computation of the electromagnetic behavior of a structure is of crucial importance for the design and operation. The electromagnetic properties of the structure depend on its geometry, which, for real-life radio-frequency (RF) structures, generally deviates from their design values due to fabrication tolerances and operation. To make assessments about the effects of such deviations as well as to employ robust optimizations, a so-called uncertainty quantification (UQ) is applied. For large and complex structures such computations are heavily demanding and cannot be carried out using standard brute-force approaches. In this paper, we propose a combination of established techniques to perform UQ for long and complex structures, where the uncertainty is located only in parts of the structure. As exemplary structure, we investigate the third-harmonic cavity, which is being used at the FLASH accelerator at DESY, assuming an uncertain geometry of the left higher order mode coupler. The investigation is carried out using the so-called polynomial chaos expansion (gPC). For that, the repeated numerical solution of Maxwell's equations is necessary. Usually, such investigations are carried out on supercomputers or small computer clusters with heavily parallelized code. Due to the fact that maximum-performance computational infrastructure is scarce and expensive, the electromagnetic properties are being computed on standard workstation computers using a newly proposed non-overlapping domain decomposition scheme named State-Space Concatenation (SSC) which is based on model-order reduction of the decomposed segments. Using the SSC scheme has the most important advantage that only the uncertain part of the structure, in our case the left coupler, needs to be recomputed when using a non-intrusive scheme like gPC. In comparison to the huge computational demand of a straightforward simulation, the combination of uncertainty quantification and model-order reduction allows for a reasonable improvement of the computational efficiency. Both schemes can be separately applied to structures related to accelerator physics. Yet, just their combination will enable the investigation of long and complex structures beyond the scope of standard approaches.

1. INTRODUCTION

The design of RF-structures usually does not take fabrication tolerances into account. These tolerances make the operated design uncertain. For a thorough design, the effects of the uncertain geometry regarding the RF-properties of the structure need to be assessed which is of growing interest in RF-design [1–4]. This is employed using uncertainty quantification (UQ) [5]. Usually this requires the repeated solution of Maxwell's equations [6] for the entire structure under consideration in order to compute the eigenmodes. Since in general no closed, analytical solutions can be found, numerical techniques are employed. Due to the fact that the investigated structures are large and complex, standard discretisation techniques might lead to extreme computational demands which make the investigations only feasible using supercomputers [7]. In this paper, we propose a new approach that will decrease the needed computational time for UQ by using a newly proposed non-overlapping decomposition scheme named State-Space concatenations (SSC) [8] for the repeated solution of Maxwell's equations in combination with the generalised polynomial chaos (gPC) technique.

2. UNCERTAINTY QUANTIFICATION

For design considerations, assessments about the influence of uncertainties of design values need to be made. In the literature, the influence of uncertain design parameters on output parameters is regarded as uncertainty propagation. Usually the probability density functions (PDF) of physical parameters of the designed structures (further referred to as output parameters) are quantities of interest. These ought to be computed using the estimated PDFs of the design parameters (further referred to as input parameters). UQ techniques are usually computationally demanding. Furthermore, standard approaches like Monte Carlo (MC) only converge with the square-root of the number of samples used. To overcome the poor convergence and lower the computational demand, a different approach was proposed in [9]. The main idea is to approximate the multi-dimensional, stochastical space by a set of orthogonal polynomials. The expansion coefficients for these polynomials are obtained by computing the solution of a deterministic problem for several collocation points in the stochastical space. This approach is generally referred to as polynomial chaos [10]. For a low dimensional stochastical space, hence few uncertain input parameters, the gPC might be faster than other techniques. However, for many uncertain input parameters, the method becomes more demanding than comparable, straight-forward approaches. A detailed description is beyond the scope of this article. For a complete description please refer to [10] and references therein. A more detailed comparison of the applicable techniques for UQ in RF-design, is given in [11]. For the design of accelerating structures usually the fabrication tolerances of the structure have the highest influence [16]. Important output quantities of interest are for example the resonant frequencies of certain higher order modes (HOMs) [13].

3. STATE-SPACE CONCATENATIONS

The SSC scheme employs a non-overlapping, domain-decomposition method to the investigated structure in order to compute the eigenmodes for closed structures. In a first step, the structure is decomposed into several, non-overlapping domains. For these domains a second order state space model (SSM) is computed using a model-order reduction (MOR). The SSM are then concatenated to a larger SSM which contains all the RF-parameters of the full structure in the given frequency interval. Since the concatenation of the models is relatively fast (several seconds for this application), the computational demand of the UQ is mainly governed by the recomputation of the uncertain part. Thus, compared to standard approaches, a significant decrease in the computational demand can be observed. The accuracy and suitability of the SSC scheme was proven in several publications [8, 14, 15].

4. APPLICATION EXAMPLE

As application example, a part of the third-harmonic cavity of the FLASH accelerator in Hamburg is chosen as depicted in Fig. 1. The structure consists of a superconducting 9-cell cavity, a superconducting HOM coupler (attached to the left iris of the cavity) and a HOM coupler including an input coupler (attached to the right iris of the cavity). For the application of SSC, a suitable decomposition needs to be selected. In this example, the decomposition is chosen as depicted in Fig. 2.

As a practical example, we try to investigate the effect of a geometrical uncertainty in the left HOM coupler (depicted in blue in Fig. 2). For this purpose, the depth of the antenna, as well as the distance between the coupler and the cavity are chosen to be uncertain as depicted in Fig. 3. It should be noted, that even though the uncertainty is located in the coupler, it still can influence all the eigenmodes, even when they are not solely located in the uncertain part of the structure. Both uncertain parameters are assumed to be symmetrically uniformly distributed with a

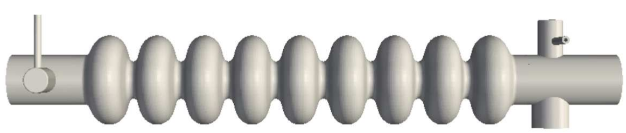


Figure 1: Qualitative plot of the third-harmonic cavity with HOM couplers and input coupler. This structure is being used in the FLASH accelerator in Hamburg at DESY [16].

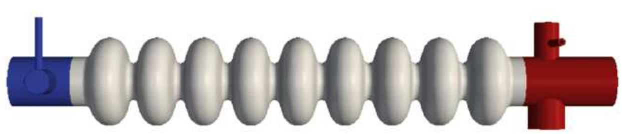


Figure 2: Decomposition of the computed structure into three parts. The blue part depicts the left HOM coupler whose geometry is considered uncertain. The white color depicts the 9-cell cavity (it should be noted that for the computation of the cavity symmetry boundary conditions can be applied since the structure is rotationally symmetric). The red color indicates the right HOM coupler which also contains the input coupler that is used to excite the accelerating mode inside the cavity. In the application example, some geometrical parameters of the blue part are assumed to be uncertain.

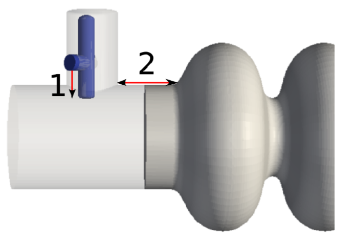


Figure 3: Segment of the full structure including the uncertain geometry parameters. The depth of the coupler antenna (depicted in blue with number 1) and the distance between the coupler and the cavity (depicted with number 2) are assumed to be uncertain.

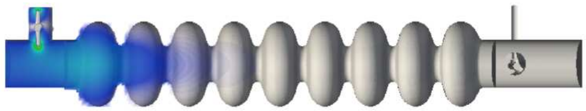


Figure 4: Qualitative plot of the magnitude of the electric field of an investigated mode at roughly 4.11 GHz. This mode is mainly located at the coupler and thus it is highly sensitive with respect to uncertainties in the said coupler in question.

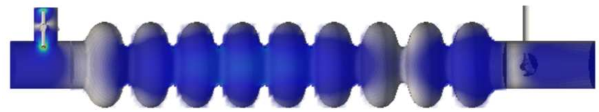


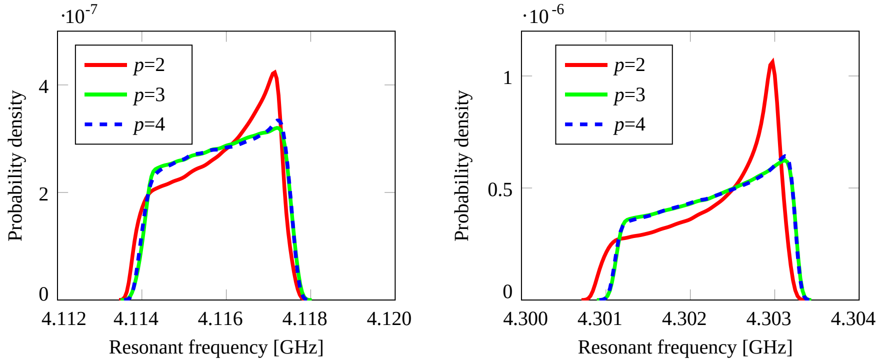
Figure 5: Qualitative plot of the magnitude of the electric field of an investigated mode at roughly 4.30 GHz. This mode is able to traverse through the entire structure but it is mainly located at the coupler. Thus it is highly sensitive to uncertainties in the coupler.

maximum deviation of 0.125 mm. Since the practical knowledge about deviations of HOM couplers is scarce, these values are assumptions based on deviations expected in the cavity and might not reflect the real-life behaviour. As result we compute the PDFs of several resonant frequencies inside the structure. In order to show the scope of the presented methods, this example is beyond the capabilities of direct approaches on standard workstation computers and by this can not be verified using standard brute force approaches. However, both methods were validated separately, in several other applications as described, e.g., in [17].

5. RESULTS

As results of the UQ, the probability density functions (PDF) of the resonant frequencies of two eigenmodes were computed using gPC using an expansion degree of up to 4. As first example the resonant frequency of some mode at roughly 4.11 GHz located inside the left HOM coupler was investigated. The field pattern computed for the certain design is depicted in Fig. 4. Due to its good coupling to the HOM coupler this mode is expected to have a strong dependence on the uncertainty of the coupler. The PDF computed using gPC is shown in Fig. 6(a). It can be seen that the difference between the computation using a polynomial degree of $p = 3$ and $p = 4$ is relatively small, hence the solution of the gPC converges. It should be noted, that this convergence only refers to the gPC. The convergence of the mesh of the deterministic problem needs to be examined beforehand. Which polynomial degree is necessary depends on the application and the finally desired accuracy. When the goal is only a rough assessment, hence only lowest-order stochastical moments, even a polynomial degree of $p = 2$ might be sufficient. For higher accuracy a polynomial degree of $p = 3$ might be needed. It should be noted, that this assessment needs to be made separately for every mode and does not need to hold for the other modes as well.

Further, the PDF of the resonant frequency of a mode at roughly 4.30 GHz was investigated. A qualitative plot of the electric field can be seen in Fig. 5. This mode has its maximum amplitude in the uncertain coupler but is able to traverse through the entire structure. In Fig. 6(b), the PDF of this mode is computed using gPC with different polynomial orders p. It can be seen that an order of $p = 3$ is sufficient in order to make assessments about the stochastical moments. As a third example the resonant frequencies of the first monopole band of the cavity were investigated which are located approximately between 3.75 GHz and 3.9 GHz. For these modes, the UQ can not be performed properly since the changes in the frequencies caused by the uncertain design, were below the actual numerical accuracy of the model (several 100 kHz). However, one can still claim that, since the changes in the frequency are below the models numerical accuracy, these modes



(a) (b)

Figure 6: PDFs of resonant frequency (a) of the mode shown in Fig. 4 at roughly 4.11 GHz and (b) of the mode shown in Fig. 5 at roughly 4.30 GHz computed using gPC with different polynomial degrees.

are barely sensitive regarding uncertainties in the coupler. The full computation of the structure using SSC takes approximately 90 minutes. However, for any collocation point of gPC, only the uncertain coupler needs to be recomputed. Hence, the recomputation of the solution for any gPC sample takes approximately 10 minutes and 30 seconds each. This results in a time for full UQ for a polynomial degree of $p = 3$ of approximately 4.5 hours for the full spectrum.

6. CONCLUSION

In this investigation, we could show the successful combination of gPC and SSC in order to employ UQ for large and complex RF-structures. Therefore, an example from accelerator physics was picked, the Third-Harmonic cavity of the FLASH accelerator. In this application, parts of the upstream HOM coupler were assumed to be uncertain regarding their geometry. Using the proposed approach, we were able to compute the PDFs of several eigenmodes as well as their low-order stochastical moments. It could be shown, that modes from the first monopole band of the cavity, are hardly influenced by the uncertainty of the coupler. However, it should be noted that for a real assessment of the PDFs of these modes, the accuracy of the model needs to be several orders of magnitude higher.

As expected, modes that have a strong coupling to the uncertain coupler are heavily influenced. In both cases a polynomial degree of $p = 3$ was necessary to quantify the standard deviation with a relative accuracy below 10^{-6}. The combination of the two techniques allows for investigations on workstation computers instead of brute force approaches on high performance computers. Nevertheless, it should be mentioned that in this investigation, only parts of the structure were assumed to be uncertain, which, in real-life applications might not hold.

A reasonable claim against a full eigenmode analysis might be, that the investigation of the frequency can also be carried out using scattering parameters. However, for the tracking of a mode through the uncertain spectrum this might not be possible, because a specific mode is characterized and thus recognized by its specific field pattern while the frequency information might not be sufficient. In future investigations we will focus on the investigation of fully uncertain, large and complex structures. Further, in future investigations, the full spectrum will be investigated. For this, a decent mode recognition needs to be implemented as in, e.g., [18].

ACKNOWLEDGMENT

The authors would like to thank the BMBF Germany for sponsoring this work under contract number: 05K13HR1, as well as the EuCARD-2 Project, cofunded by the European Commission 7th in Framework Programme.

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