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Physics Procedia 79 (2015) 38 – 45

Physics Procedia

ICFA mini Workshop on Higher Order Modes in Superconducting Cavities, HOMSC14

Computational benefits using an advanced concatenation scheme based on reduced order models for RF structures

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Abstract

The computation of electromagnetic fields and parameters derived thereof for lossless radio frequency (RF) structures filled with isotropic media is an important task for the design and operation of particle accelerators. Unfortunately, these computations are often highly demanding with regard to computational effort. The entire computational demand of the problem can be reduced using decomposition schemes in order to solve the field problems on standard workstations. This paper presents one of the first detailed comparisons between the recently proposed state-space concatenation approach (SSC) and a direct computation for an accelerator cavity with coupler-elements that break the rotational symmetry.

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Peer-review under responsibility of the Fermi National Accelerator Laboratory

Keywords: Numerical techniques, model order reduction, eigenvalue problems, wideband equivalent model, accelerator physics.

1. Introduction and Motivation

The design and investigation of RF structures for particle accelerators is often a challenging task. For this purpose, numerical simulations are performed which allow for the full description of the structures' electromagnetic properties in the frequency interval of interest (usually several GHz) as well as in time domain. Important properties of RF structures which need to be determined by the numerical codes are e.g. scattering or impedance parameters or the eigenmodes. They form a complete set of orthogonal, harmonic functions which characterize the electromagnetic behaviour of the RF structure.

Often numerical computations are executed in parallel on supercomputers as described p.e. by Lee et al. (2009). However, the access to these computing infrastructures is limited. Furthermore, computational time on supercomputers is not always available and users can spend a vast amount of time in pending queues. Therefore, it might be reasonable to reduce the computational demand for the computations by using a so-called decomposition scheme. Here, the complex RF structure is decomposed into several, less complex RF structures. The electromagnetic properties of these substructures are computed and then, from the results, a model of the RF properties of the full structure is derived. Thus, it can be achieved that the computations can be carried out on workstation computers. In particular for large RF structures, decomposition schemes result in computational benefits and substantially reduce the computa-

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doi:10.1016/j.phpro.2015.11.060

tional demand. Moreover, ill-conditioned linear equation systems can be avoided since the numerical systems arising from the decomposition are smaller and have smaller condition numbers. A further benefit when using decomposition schemes goes along with a proper decomposition. Some examples are given here: In some cases, the structure can be decomposed in such a way that symmetry boundary conditions are applicable for one or several segments which further reduces the computational effort. For repetitive structures, the computed models might well be used several times. When dealing with rotational-symmetric substructures also 2D-solvers are applicable. Eventually some substructures can even be treated analytically.

Literature proposes many different approaches for the decomposition of RF structures in order to speed up and/or enable certain computations. All methods have their individual advantages and drawbacks. There are mode-matching techniques described by Shinton et al. (2012), van Rienen (1993) and Wessel et al. (1999). These methods provide the field information but they have hard requirements on the shape of the structures and are difficult to apply for arbitrary topologies. Further there are several publications on techniques purely based on the scattering parameters by Glock et al. (2002) and Bane et al. (2009) and on other methods based on a decomposition in electric circuits by Liepe (2001) and Wittig et al. (2006). All frequency-domain methods have in common that the field information is lost in the concatenation because they operate with integral quantities. However, resonant frequencies and field distributions of eigenmodes are deducible by the frequency-domain transfer functions of the segments with techniques described by Rothemund et al. (2001). This has the drawback that narrow bands containing many eigenmodes need a very dense sampling in the frequency domain which might result in long computational times. Thus, these computations might only be advantageous when dealing with few modes. Therefore, they might be an option when investigating effects of certain eigenmodes or small bands of eigenmodes but not effects in frequency ranges where no a priori knowledge is available about the specific eigenmodes which contribute to the investigated effects.

To overcome the above-mentioned drawbacks, the investigations carried out in this paper use a recently proposed decomposition scheme, denoted as state-space concatenations (SSC) introduced by Flisgen et al. (2013). In contrast to all of the techniques mentioned before, SSC provides a decomposition in which all RF properties are preserved in a wide frequency range and fast investigations in time domain, as well as in frequency domain are possible for arbitrary topologies and decompositions. This will allow for the fast computation of eigenmodes, as well as scattering and impedance parameters of large and complex structures. In addition, the scheme does not rely on a certain numerical technique to treat the RF properties of the decomposed segments. Furthermore, the method is not limited to RF structures but could be applied to any arbitrary closed structure in which the electromagnetic fields need to be computed.

This method has been applied with great success to several simple RF structures by Flisgen et al. (2012) as well as for large structures with rotational symmetry by Flisgen et al. (2014). The aim of this study is to describe and quantify the numerical benefits and the accuracy of SSC for an exemplary structure which breaks the rotational symmetry, in order to show the advances over the direct approach.

2. Theory

The work presented in this paper is based on the theory derived by Flisgen et al. (2013). For the sake of completeness, the main ideas are briefly revised in this section. The aim of the scheme is the fast computation of the RF properties of a structure in a certain frequency interval. This is accomplished by decomposing the structure into several segments. The locations where the structure is split are afterwards denoted as cutting planes. For each segment a reduced order model is generated. Subsequently, all reduced order models are concatenated to a reduced model of the full structure. This model retains all RF properties of the full structure in the frequency range of interest.

This aim is accomplished by the description of structures and substructures using so-called second-order state-space models. For the rth segment they are given by:

$$\begin{aligned} \frac{\partial^2}{\partial t^2}\mathbf{x}_r(t) &= \mathbf{A}_r\,\mathbf{x}_r(t) + \mathbf{B}_r\,\frac{\partial}{\partial t}\mathbf{i}_r(t), \\ \mathbf{v}_r(t) &= \mathbf{B}_r^{\mathrm{T}}\mathbf{x}_r(t). \end{aligned} \tag{1}$$

Here, $\mathbf{A}_r$ denotes the state matrix, $\mathbf{B}_r$ the input matrix and $\mathbf{B}_r^{\mathrm{T}}$ the output matrix of the rth segment and $\mathbf{x}_r(t)$ the inner states of the system. Theses state-space models are of relatively small order (several hundred degrees of freedom) compared to state-space models arising from the full discretisation of the segments using an appropriate numerical formalism (several million degrees of freedom) like the finite element method (FEM) described by Rylander et al. (2013) or the finite integration technique (FIT) described by Weiland (1977) and Weiland (1996).

For the derivation of these state-space models of the substructures, the electromagnetic properties of the segments are required. Namely the 3D eigenmodes of the single segments, the 2D eigenmodes of the cutting planes and of the port surfaces are needed. The reduced model is then generated from the resonant frequencies of the eigenmodes, as well as the interaction integrals of the 3D eigenmodes of the structure and the 2D eigenmodes at the cutting planes and at the port surfaces. Note that these are only surface integrals since the 2D eigenmodes vanish everywhere but in the port/cutting-plane surfaces. An appropriate choice of the number of considered 2D port modes, as well as 3D eigenmodes is important for the accuracy of the method. For the 2D port/cutting-plane modes, at least every 2D mode which is able to propagate in the frequency interval of interest needs to be considered. This means that its cutoff frequency needs to be below the upper boundary of the considered frequency interval. For the 3D eigenmodes, at least every mode whose resonance frequency lies in the frequency interval of interest should be considered. In practice, the 3D eigenmodes with resonant frequencies outside the given frequency range have a non-negligible influence. They are accounted for, by computing the field distribution resulting from the excitation at the ports with a certain frequency. These field distributions are computed for a number of samples and afterwards an orthogonal decomposition is applied. For obtaining an impedance formulation using state-space systems, all waveguide ports of the single segments have to be terminated with perfect magnetic conducting material (PMC). For the concatenated, full model, different boundary conditions, like perfect electric conducting (PEC) or open boundary conditions, can be simulated in a cheap post-processing step as derived by Flisgen et al. (2014).

After the computation of the state-space models of the substructures, they need to be concatenated to the state-space model of the full structure. It is important to notice that this model condenses all important electromagnetic properties of the structure in the chosen frequency interval. The concatenation is done by matching the modal port currents and modal port voltages at the cutting planes. With the obtained reduced order model of the full structure, time domain investigations are possible by simply solving the system of ordinary differential equation for given inputs. Also frequency-domain properties are easily obtained by computing e.g. the transfer function of the system. Note that these operations have comparably low numerical costs since the state-space system has relatively few degrees of freedom.

3. Model Structure and Implementational Aspects

A three-cell cavity including higher order mode (HOM) couplers and a power coupler is chosen as an application example (see Fig. 1). It is important to note that this structure shows no symmetry of any kind which could reduce the computational effort while computing its RF properties. That is why in many cases the couplers are left out of the computation in order to apply symmetry boundary conditions to the cavity as stated by Shinton et al. (2012). However, this does not allow for a fully realistic study of the electromagnetic behaviour of the structure or the behaviour of the coupler.

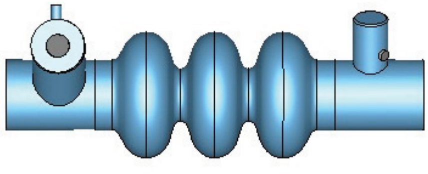

Fig. 1. Elliptical three-cell cavity (middle) with HOM coupler (left) and HOM- and power coupler combination (right).

Since the numerical treatment of such structures is of crucial importance for the understanding of the functionality of accelerating structures it is an appropriate real-life example. On the one hand, the structure shows a complexity which allows no further reduction (like symmetry boundary conditions) nevertheless, we are still able to validate the results by computing it using a direct approach. In real-life examples, the structures might be much longer and typically consist of chains of several structures. The aim of this study is to quantify the numerical benefits from the proposed scheme in comparison to the full, straightforward computation of the structure using CST Microwave Studio® (CST MWS (2014)). This software tool is a standard for numerical computation of electromagnetic fields in science as well as in the industry using FIT and FEM.

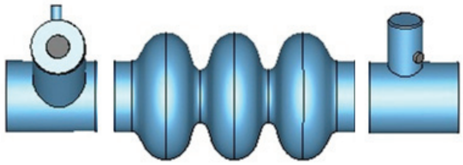

Fig. 2. Decomposition of the full structure (refer to Fig. 1) into three single segments.

In a first step, the structure is subdivided into three segments, which are: the left HOM-coupler with beam pipe (left), the three-cell elliptical cavity (middle) and the right HOM-coupler with beam pipe and power coupler (right), as depicted in Fig. 2. For simplicity reasons, PEC boundary conditions are assigned to the waveguide port facets of the power coupler. Theoretically, the decomposition is arbitrary regarding the cutting planes as well as the numbers of segments. However, the depicted decomposition has certain advantages: Firstly, one can pick two relatively small parts, in this case the two couplers. Also, the third part, the cavity, allows for a speed-up due to the fact that it is symmetric to its mid plane so that symmetry boundary conditions are theoretically applicable and by this the computational demand can be lowered substantially. However symmetry-boundary conditions were not applied in this paper. Theoretically, the 2D treatment of the cavity would also be possible due to its rotational symmetry regarding the beam axis. However, due to the lack of a 2D eigenmode solver in CST MWS this was not further investigated.

For the case shown here, there are five 2D modes that need to be considered at the cutting planes on the beam pipe between the segments. As waveguide port modes, the TEM mode has been chosen at the outer planes of the two HOM couplers.

The single segments are meshed in CST MWS and the 2D port modes are computed. From this computation the system matrix, the 2D port modes and the mesh are exported to Matlab (2013) where the state-space systems are obtained according to Flisgen et al. (2013). Due to the fact that only hexahedral meshes can be exported in CST MWS, all computations were carried out with a hexahedral mesh (for hexahedral meshes CST MWS uses FIT). In table 1 the resulting number of mesh cells as well as the number of 3D and 2D eigenmodes are displayed.

Table 1. Numerical aspects of individual segments in CST MWS.

Part	**Mesh Cells**	**3D Eigenmodes**	**2D Eigenmodes**
Left HOM coupler	162, 792	79	11
Right HOM coupler with power coupler	274, 856	178	11
Cavity	126, 960	112	10

4. Results

In this section, the results will be shown and quantified. All of the computations have been performed in a frequency range of 0 to 8 GHz on a Intel(R) Xeon(R) CPU E5-2687W @ 3.4 GHz with 256 GHz of RAM. Table 2 shows the computational time needed for the application of the SSC scheme.

It becomes obvious that the coupling of the reduced models takes minor time compared to the actual computation of the reduced order state-space models for the segments.

Table 2. Computational time for state-space systems

Computation with SSC	**Computational time needed**
Left HOM coupler	28 min 26 s
Right HOM coupler with power coupler	55 min 06 s
Cavity	32 min 31 s
Coupling of all	12 s
Full SSC computation	1h 56 min 15s

4.1. Impedance Parameters

For the investigated structure, the impedance parameters were computed by employing the transfer-function of the SSC model. For validation purposes it has also been computed directly using CST MWS having (roughly) the same spatial discretisation. The resulting impedance parameters are displayed in Fig. 3.

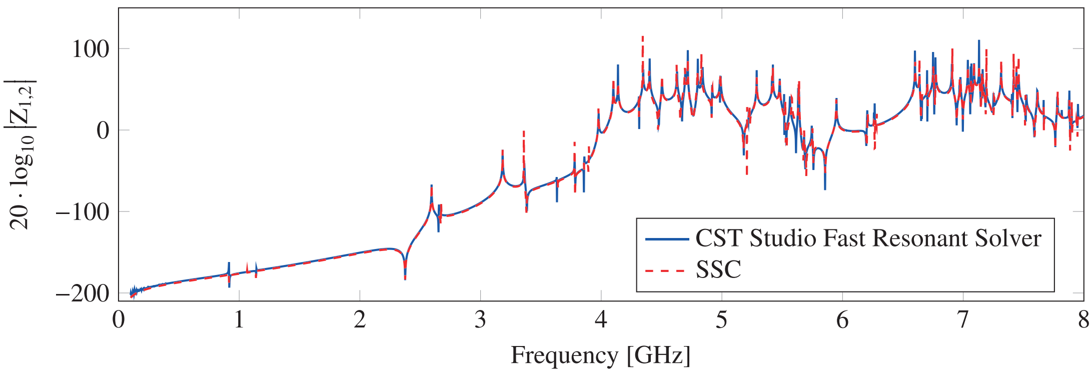

Fig. 3. Impedance parameter $Z_{1,2}$ (transmission from the left HOM coupler to the right HOM coupler) computed with SSC (red curve) and CST MWS Fast Resonant Solver (blue curve).

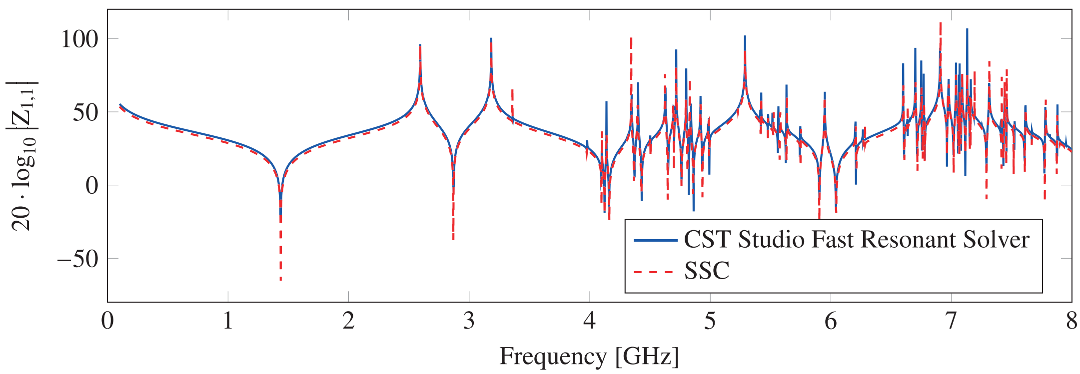

Fig. 4. Impedance parameter $Z_{1,1}$ (reflection on the left HOM coupler) computed with SSC (red curve) and CST MWS Fast Resonant Solver (blue curve).

In Fig. 3 the transmission from the left HOM coupler to the right HOM coupler is shown. It can be observed that both results agree well in the full frequency range. The same holds for the reflection on the left HOM coupler as displayed in Fig. 4. For the impedance parameter computation, CST MWS took 2 hours 1 minute and 6 seconds, which is roughly the same as the application of the SSC scheme. This suggests that, when investigating the impedance parameters, the application of the scheme is not beneficial in general but only for structures of a higher complexity than this rather simple structure.

4.2. Eigenmodes

From the concatenated SSC model the eigenmodes of the full structure can be derived. For comparison, the 3D eigenmodes were computed using CST MWS with roughly the same spatial discretisation. The direct solutions were obtained by discretising the problem using FIT and solving it with the Jacobi-Davidson method as described by Sleijpen et al. (1996) and Sleijpen et al. (2000). The relative difference from the SSC solution to the CST MWS solution, regarding the resonant frequencies of the eigenmodes, are shown in Fig. 5.

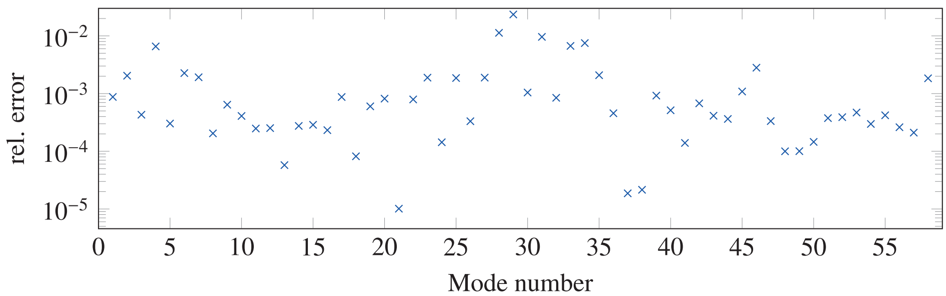

Fig. 5. Absolute, relative difference regarding the resonant frequencies of the eigenmodes when comparing CST MWS and SSC.

It can be seen that the two compared schemes compute roughly the same resonant frequencies of the eigenmodes. The relative difference has a mean of $9.6601 \cdot 10^{-4}$. For this computation, the computational time required using SSC is substantially lower than that of CST MWS. While the complete SSC computation took 1h 56 min 15s , CST MWS took 287 hours, 38 minutes and 59 seconds.

5. Discussion and Outlook

In this paper, the computational time and the accuracy regarding impedance parameters and eigenmodes have been compared for the computation of a three-cell cavity including HOM- and power couplers. The impedance parameters as well as the eigenmodes are computed using SSC for the segmented structure and a direct approach using CST MWS for the full structure. It could be shown, that both results match relatively well compared to the CST MWS results for the full structure. In the chosen spectrum from 0 - 8 GHz the resonant frequencies of the eigenmodes have a mean relative difference of $9.6601 \cdot 10^{-4}$, whereas the computational time of the problem is reduced to approximately 0.7 % with the SSC approach. For a longer structure like the full string of third harmonic cavities these effects will be even larger, since already computed parts can be used several times. Also, the superiority of the proposed scheme over already existing schemes using a frequency-domain coupling has become obvious since the SSC method is able to compute eigenmodes in broad frequency intervals. Nevertheless, it is important to say that using the examined scheme might be only appropriate when investigating all eigenmodes in a broad frequency range. Otherwise frequency-domain methods might be more suitable. In further investigations the method is being employed to compute the eigenmodes of the full chain of four cavities for the FLASH third harmonic module described by Sekutowicz et al. (2002), and the chain of eight cavities for the XFEL. The capability of the method for such long, rotationally symmetric structures was shown by Flisgen et al. (2014). This enables investigations far beyond the scope of direct computations on standard workstation. Some results are shown in Fig. 6 for the XFEL third-harmonic cavity chain, without the input- and HOM couplers. The plot is obtained using Paraview (Userguide written by Henderson et al. (2004)).

In order to quantify the effects of geometric uncertainties for such structures we will perform several parameter studies with these structures. For this, the proposed scheme is especially suitable and it will allow us in the first place to do such simulations since such parameter studies have a huge computational demand that would not allow for a

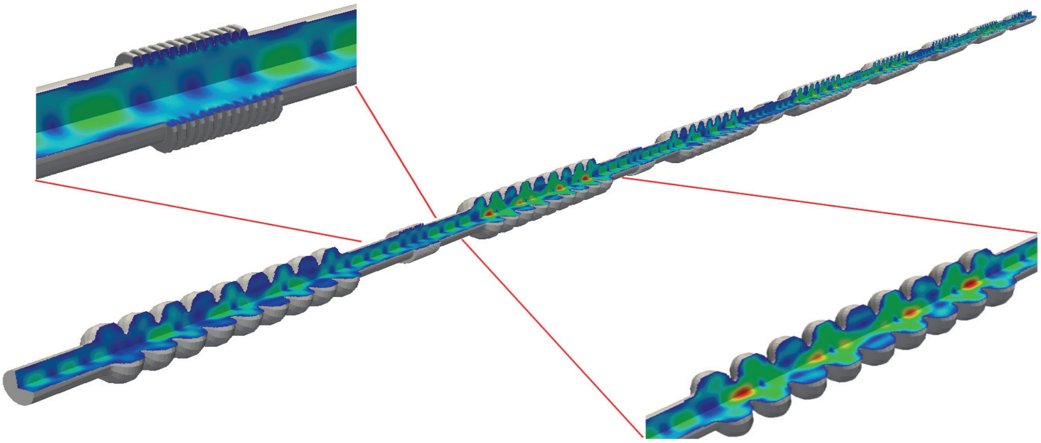

Fig. 6. Magnitude of the electric field of a higher order multi-cavity eigenmode in a chain of eight superconducting 3.9 GHz cavities (zoom at the bottom), which are connected via beam pipes and bellows (zoom at the top).

direct computation in reasonable time. Further, the SSC scheme will be combined with uncertainty quantification for RF structures as carried out by Heller et al. (2014) and Schmidt et al. (2014).

Acknowledgements

The authors would like to thank the BMBF Germany (contract number 05K13HR1) and the EuCARD-2 Project, cofunded by the European Commission 7th in Framework Programme for the financial support of this work. Further, we would like to thank C. Bahls for fruitful discussions about performance constraints and F. Reimann for her help regarding Paraview.

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