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IMPEDANCE COMPUTATION FOR LARGE ACCELERATOR STRUCTURES USING A DOMAIN DECOMPOSITION METHOD* †

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Abstract

We introduce a domain decomposition technique for impedance computations in the frequency domain. The technique allows to handle large accelerator structures by decomposing the computational domain into smaller subdomains, which interact by means of suitably chosen boundary conditions. We describe a class of such boundary conditions that can accurately reproduce the full-scale electromagnetic field solution in the presence of a particle beam. As an important application of the method we consider the impedance characterization of a large in-vacuum undulator for the PETRA IV synchrotron radiation source.

INTRODUCTION

The computation of beam coupling impedances is a crucial step in the design and optimization of particle accelerators. Traditionally, this task has been accomplished by employing so-called wakefield solvers, which essentially solve Maxwell's equations in the time domain for ultra-relativistic beams [1]. However, this approach is not well suited for highly resonant structures. Additionally, the approximation of complex geometries remains a challenge for the Finite-Difference-type technique used in these solvers.

We have recently proposed a simulation methodology for computing beam impedances directly in the frequency domain (cf. [2]). The method produces highly accurate results, when appropriate mixed-element meshes adapted to the particle-beam problem are employed. Hereby, the bottleneck is the lack of scalable algebraic solvers for the large system of algebraic equations resulting from Finite Element (FE) discretizations. In order to tackle the problem, an impedance concatenation technique based on domain decomposition and a set of generalized S-Parameters (CSC$^{\mathrm{BEAM}}$) has been proposed [2]. This method requires the computation of a full S-Parameter matrix for each of the subdomains. Most of this information is superfluous, since not all of the electromagnetic modes exited in the chamber contribute to the beam impedance. Therefore, CSC$^{\mathrm{BEAM}}$ often leads to unnecessarily long simulation times.

In this work, we propose a new Domain Decomposition Method (DDM) based on the non-overlapping Schwarz approach [3]. This method does not require explicit S-parameter extraction. We exploit the waveguide-like structure of the accelerator problem to develop a class of specialized boundary conditions for the subdomain interfaces leading to fast numerical convergence. Using this technique we perform the full impedance characterization of an In-Vacuum Undulator (IVU) for use at the PETRA IV synchrotron radiation source at DESY, Hamburg [4].

THE IMPEDANCE PROBLEM

The electromagnetic fields in the frequency domain are described by the time-harmonic Maxwell's equation

$$\nabla \times \nabla \times E - k_0^2 E = -ik_0 Z_0 J(r,\omega), \tag{1}$$

where E is the electric field, $k_0 = \omega/c$ with ω the frequency, J is the source current density and Z_0, c are the vacuum impedance and the speed of light in vacuum, respectively. The current density corresponding to an ultra-relativistic particle of charge q moving in the z-direction at a traverse position $r_\perp^{(1)}$ is given by

$$J(r_\perp^{(1)}; r,\omega) = q\delta(r_\perp - r_\perp^{(1)})e^{-ik_0 z}. \tag{2}$$

The longitudinal coupling impedance to a witness particle with a potentially different transverse offset at $r_\perp^{(2)}$ is

$$Z_\parallel(r_\perp^{(1)}, r_\perp^{(2)};\omega) = -\frac{1}{q^2}\int \mathrm{d}^3 r J^*(r_\perp^{(2)}; r,\omega) E(r_\perp^{(1)}; r,\omega), \tag{3}$$

where $E(r_\perp^{(1)}; r,\omega)$ denotes the electric field excited by the source particle at $r_\perp^{(1)}$. Transverse coupling impedances can be derived from (3) using Panofsky-Wenzel theorem [5]. Furthermore, by careful analysis of the resulting impedance spectra it is possible to determine the resonance frequencies of the chamber as well as the corresponding shunt impedances and Q-factors as described, e.g., in [6].

Finite Element Model

For the numerical solution of (1), we employ a high-order FE approach. Given a discretization of the computational domain, Ω, the electric field is approximated on a tangentially continuous $H(\mathbf{curl})$-space defined on the mesh [7]. Then, following standard procedure the weak form of (1) is

$$\begin{aligned}\left(\nabla\times\phi_h, \nabla\times E\right)_\Omega - k_0^2\left(\phi_h, E\right)_\Omega = \\ -ik_0 Z_0\left(\phi_h, J\right)_\Omega - \left(\phi_h, n\times\nabla\times E\right)_{\partial\Omega},\end{aligned} \tag{4}$$

$\forall \phi_h \in H(\mathbf{curl})$, where $(\cdot,\cdot)$ denotes scalar-product. The last surface integral term in (4) needs to be treated according to the specific boundary conditions on $\partial\Omega$. In the following, we are less interested on the implementation of (4) for

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general boundary conditions. For this, we refer the reader to a forthcoming publication. However, important for the present discussion is the handling of the boundary term at the input and output pipes, where the particle beam enters and exits the computational domain, respectively.

Beam Ports

We assume that the cavity structure is connected to an incoming (or outgoing) pipe of infinite length along the z-direction at some position z_Γ. We refer to the cross-section, $Gamma \subset \partial Omega$, of the pipe at z_Γ henceforth as a beam port. The total field on Γ is,

$$E|_\Gamma = E_{\text{inc}}|_\Gamma + \sum_k \left(e_k^{\text{TX}}, E - E_{\text{inc}}\right)_\Gamma e_k^{\text{TX}}, \qquad (5)$$

where e_k^{TX} are waveguide modal functions with TX standing for the TE-, TM- and TEM-modes supported by the pipe. The incoming field, E_{inc}, describes the stationary electric field of an incoming (or outgoing) particle of constant energy propagating in the infinite pipe. In the ultra-relativistic case, this field is given by the solution of

$$\nabla_\perp \cdot E_{\text{inc}} = \frac{q\delta(r_\perp - r_\perp^{(1)})}{c\varepsilon_0} e^{-ik_0 z_\Gamma}, \quad \nabla_\perp \times E_{\text{inc}} = 0, \quad (6)$$

on Γ, where the charge density corresponding to the particle current (2) at $z = z_\Gamma$ has been used. Given a solution of (6), we express the boundary term in (4) by means of (5) to obtain

$$\left(\phi_h, n \times \nabla \times (E - E_{\text{inc}})\right)_\Gamma = P_\Gamma(E - E_{\text{inc}}). \qquad (7)$$

The weak port operator, P_Γ, is defined in terms of waveguide modes according to

$$P_\Gamma(E) = \sum_k \gamma_k^{\text{TX}} \left(\phi_h, e_k^{\text{TX}}\right)_\Gamma \left(e_k^{\text{TX}}, E\right)_\Gamma, \qquad (8)$$

where γ_k^{TX} are modal propagation constants.

Equation (4) together with (7) and (8) is fully sufficient to formulate the discrete impedance problem for arbitrary beam excitations. We have previously employed this approach, e.g., in [2] and [6] to compute the impedance of various accelerator structures with complicated 3D-geometry. Hereby, the main challenge is the large computational effort associated with size of the discrete problem, which commonly involves tens of millions of unknowns.

DOMAIN DECOMPOSITION METHOD

The idea consists in splitting the computational domain into subdomains along the beam path as illustrated in Fig. 1. Applying FE discretization in each of the subdomains, results in a set of discrete problems of substantially smaller size than for the full geometry. Furthermore, the subdomain problems can be solved on different computers, thus, providing a natural way to parallelize computations.

The global solution, however, must ensure the continuity of electric fields at domain interfaces. In the non-overlapping

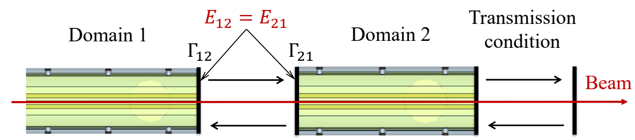

Figure 1: Schematics of a simple domain decomposition into two subdomains. The interface between the subdomains is described by the planar boundaries Γ_{12} and Γ_{21}.

Schwarz DDM approach, this is realized by iterating the individual subdomain solutions using appropriate boundary conditions at the subdomain interfaces. In the DDM context, these boundary conditions are often referred to as transmission conditions [3]. Various such conditions for the time-harmonic Maxwell's equations have been proposed in the literature [8]. In the general case, however, the numerical convergence of the DDM iteration is not guaranteed.

Modal Transmission Condition

In the specific case of impedance problems, we may exploit the typical accelerator setting, which consists of a string of cavities and waveguide-like structures that are arranged successively along the beam line. In every step of the DDM iteration, the *exact* boundary condition at the interfaces can be formulated in term of waveguide modes. Referring to Fig. 1, the Modal Transmission Condition (MTC) in Domain 1, on interface Γ_{12} follows directly from (7) by replacing $E_{\text{inc}} \to E_{21}$, where E_{21} is the solution provided by Domain 2 at the interface:

$$\begin{aligned} P_{\Gamma_{12}}(E_{12}) - \left(\phi_h, n_{12} \times \nabla \times E_{12}\right)_{\Gamma_{12}} &= \\ P_{\Gamma_{21}}(E_{21}) + \left(\phi_h, n_{21} \times \nabla \times E_{21}\right)_{\Gamma_{21}} &:= F_{12}. \qquad (9) \end{aligned}$$

In (9), we have introduced the boundary flux, F_{12}, on Γ_{12} as seen from Domain 1. For a fixed-point iteration based DDM this condition leads to the simple update scheme for the boundary fluxes,

$$F_{12}^{n+1} = -F_{21}^n + 2P_{\Gamma_{21}}(E_{21}^n). \qquad (10)$$

In practical computations, more efficient Krylov subspace iterative solvers can be used, thus, resulting in substantially less iterations than for the fixed-point scheme. Also, since the incoming field of the particle beam, E_{inc}, is the same on both sides of the interface, it is sufficient to apply the transmission condition (9) on the scattered part of the field only, corresponding to the wakefield in the cavity.

Validation

To validate the method, we consider the impedance of a lossy, rectangular pillbox-cavity (cf. Fig. 2). A two-domain decomposition is applied by splitting the cavity vertically in the middle of the resonator. Figure 2 shows the computed longitudinal impedance about the lowest resonance. The DDM result shows excellent agreement with the numerical solution obtained by a monolitic direct solver, which is applied on the full structure.

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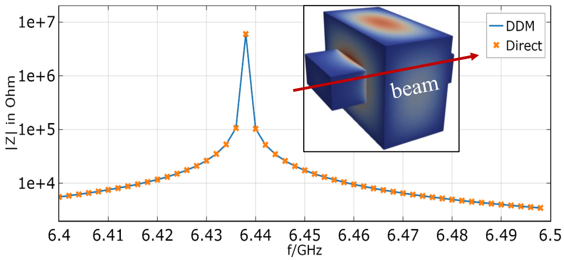

Figure 2: Lossy pillbox-cavity exited by a central beam. The longitudinal impedances computed with the DDM and a direct solver, respectively, are shown.

Figure 3 illustrates the efficiency of the method when using a GMRES iterative solver. The field distribution inside the cavity for a resonant excitation is shown at four different iteration stages. In the first two iterations, there is barely a visible interaction between the beam and the cavity. After no more than five iterations, however, the DDM procedure converges to the expected solution.

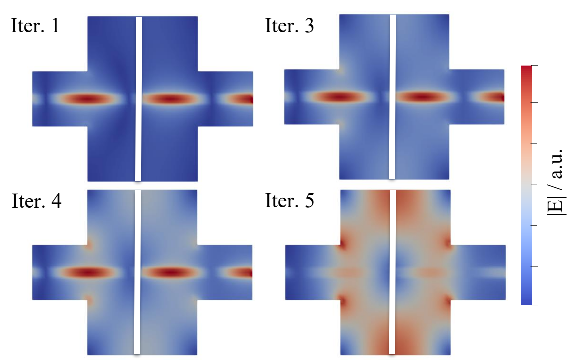

Figure 3: Progression of the DDM iteration for the lossy cavity. The electric field distribution at four different iteration stages is shown.

IVU FOR PETRA IV

In the following, we apply the DDM approach for the impedance computation of a prototype IVU for use in the upcoming synchrotron radiation source, PETRA IV at DESY. The IVU chamber supports several high-Q, trapped modes in the low frequency spectrum up to about 1 GHz, which may trigger beam instabilities [9]. We will not discuss details of the IVU as we have thoroughly done so before in [6]. An overall view of the 4.6 m-long chamber geometry is shown in Fig. 4. Also in the Figure, we visualize the decomposition of the structure into 8 subdomains of approximately the same size as used in the DDM simulation.

In the simulation, we use a finite element mesh which contains about $7 \cdot 10^5$ volume elements. Furthermore, a 4^{th}-order approximation is applied within each element. This results in nearly $40 \cdot 10^6$ total unknowns, which are distributed among 8 independent compute nodes. Hereby, each subdomain is assigned to a separate node on a HPC cluster.

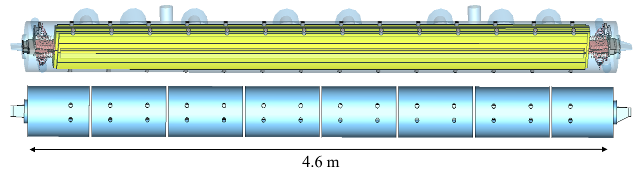

Figure 4: Vacuum chamber of the IVU (top). DDM decomposition of the geometry into 8 subdomains (bottom).

The resulting, impedance spectrum up to about 800 MHz is shown in Fig. 5.

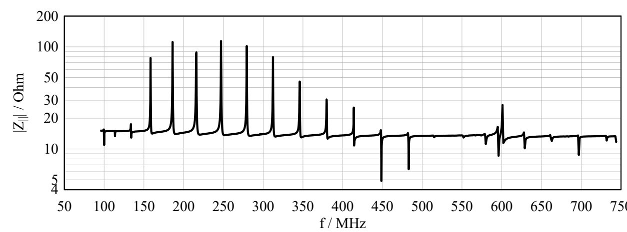

Figure 5: Impedance spectrum of the IVU computed with DDM using a frequency resolution of 0.25 MHz.

It is possible to extract the impedance from time-domain simulations with the CST wakefield solver [10]. In Fig. 6, we compare the spectra obtained with CST and DDM for the first few resonances. Clearly, both results fit very well. However, in order to reach the necessary frequency resolution for the high-Q resonant modes of the chamber, a simulation time of more than one week was needed by the CST solver. In contrast, the DDM approach allows to reduce the simulation time down to a few hours.

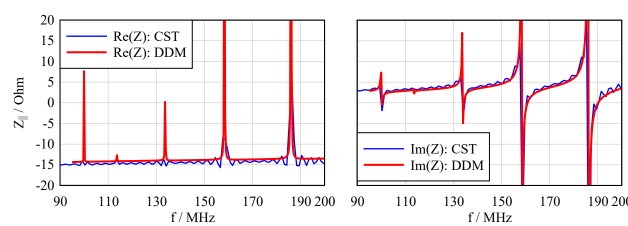

Figure 6: Comparison of the impedance spectra obtained by CST and DDM simulations.

CONCLUSION

We describe a numerical method to compute the impedance of accelerator structures in the frequency domain. Hereby, the novel contribution is a highly efficient domain decomposition approach that is tailor-suited to beam impedance problems. This approach is based on a class of modal transimission conditions that are incorporated into the Schwarz's domain decomposition framework. We have demonstrated the accuracy of this approach as well as its numerical efficiency when applied to large scale impedance problems, as is the case for the IVU at PETRA IV.

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