Time Domain Boundary Element Analysis of Wake Fields in Long Accelerator Structures

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Abstract—We present an explicit Time Domain Boundary Element Method (TDBEM) scheme with moving window technique for short-range wake field simulations of long accelerator structures. The proposed scheme is formulated by Kirchhoff’s boundary integral equation of the scattered electromagnetic field in interior region problems. Implementation of a moving window technique in the framework of TDBEM is achieved by taking into account the causality and the retardation properties of the boundary integral equation. A parallelization algorithm for this moving window implementation is also proposed. The proposed TDBEM code with the moving window technique is applied to several practical examples of long accelerator structures. Numerical results obtained with the TDBEM code are compared with those of several finite integration codes.

Index Terms—Boundary element method, moving window, parallelization, scattered fields, short-range wake field.

I. INTRODUCTION

MANY advanced accelerator projects such as linear colliders and linac-based X-ray free electron lasers require very short and high-intensity electron bunches. As the intensity is increased, the wake field [1], which is excited by electromagnetic interactions between a beam of charged particles and its surrounding environment such as accelerating cavities, becomes stronger, and consequently it can cause energy spread and emittance growth. In order to predict such harmful effects to the bunch and its surrounding environment such as accelerating cavities, modeling of arbitrary 3-D geometries and treatment of a bunch of charged particles with curved trajectories. However, most of the previous TDBEM schemes have three severe drawbacks from a computational point of view: late-time numerical instabilities, heavy calculation, and large memory requirements. For the problem of numerical instabilities stable time domain schemes were recently proposed [3]–[6]. The calculation cost problems are still serious, in particular, for short bunch wake field simulations of long accelerator structures as appeared in practical accelerator designs, although a parallelization algorithm suitable for the TDBEM schemes was presented [7]. The calculation time and the required memory of the parallelized TDBEM codes become unacceptable for such large scale problems, even if a supercomputer is available.

As is well-known in the development of wake field simulation codes, it is possible to dramatically reduce the calculation costs for a time domain wake field computation by utilizing the indirect wake potential integration [8]–[11] and the moving window technique [12]. In fact, these techniques have been applied to FIT codes.

The main purpose of this paper is to introduce a moving window technique in the framework of TDBEM. In addition, the implementation of indirect wake potential integrations in TDBEM is briefly summarized. A newly developed TDBEM code with moving window technique is applied for dispersion-free time domain wake field simulations of a short bunch in long accelerator structures.

II. SCATTERED-FIELD FORMULATION OF TDBEM

At the first part of this paper, the scattered field formulation of TDBEM is summarized for later reference. In general, the total electromagnetic fields \( \mathbf{E}, \mathbf{B} \) are explicitly split into the bunch self-fields in free space \( \mathbf{E}_{\text{self}}, \mathbf{B}_{\text{self}} \) and the scattered fields \( \mathbf{E}_{\text{scat}}, \mathbf{B}_{\text{scat}} \):

\[
\mathbf{E} = \mathbf{E}_{\text{self}} + \mathbf{E}_{\text{scat}}, \quad \mathbf{B} = \mathbf{B}_{\text{self}} + \mathbf{B}_{\text{scat}}.
\]

The bunch self-fields can be then given analytically or calculated numerically. Only the scattered fields are numerically...
solved by a TDBEM scheme which is based on the retarded Kirchhoff’s boundary integral equation of scattered electromagnetic fields on interior region problems. As described in [4], this scattered field formulation makes it easy to set up the initial fields on interior region problems and provides very stable time domain simulations even for small time step size.

Now we consider electromagnetic scattering problems on an interior region surrounded by the surface $S$ of an accelerator structure. The scattered fields $\mathbf{E}_{\text{scat}}$ and $\mathbf{H}_{\text{scat}}$ can be described by the following time domain Kirchhoff’s integral representations of scattered electric and magnetic field on interior problems with homogeneous material constants $\varepsilon, \mu$ [4]:

$$\mathbf{E}_{\text{scat}}(\mathbf{r}, t) = -\frac{1}{4\pi} \int_S \left\{ \left( \mathbf{n}' \times \mathbf{E}_{\text{scat}}(\mathbf{r}', t') \right) \times \nabla' \frac{1}{R} \right. $$

$$- \frac{1}{R} \left( \mathbf{n}' \times \frac{\partial \mathbf{E}_{\text{scat}}}{\partial t}(\mathbf{r}', t') \right) \times \nabla' R $$

$$+ \left. \left( \mathbf{n}' \cdot \mathbf{E}_{\text{scat}}(\mathbf{r}', t') \right) \nabla' \frac{1}{R} \right\} \text{d}S', \quad (1)$$

$$\mathbf{B}_{\text{scat}}(\mathbf{r}, t) = -\frac{1}{4\pi} \int_S \left\{ \left( \mathbf{n}' \times \mathbf{B}_{\text{scat}}(\mathbf{r}', t') \right) \times \nabla' \frac{1}{R} \right. $$

$$- \frac{1}{R} \left( \mathbf{n}' \times \frac{\partial \mathbf{B}_{\text{scat}}}{\partial t}(\mathbf{r}', t') \right) \times \nabla' R $$

$$+ \left. \left( \mathbf{n}' \cdot \mathbf{B}_{\text{scat}}(\mathbf{r}', t') \right) \nabla' \frac{1}{R} \right\} \text{d}S', \quad (2)$$

where $\mathbf{r}$ is the observation point in the interior region, $\mathbf{r}'$ is the position vector on the surface, $R = |\mathbf{r} - \mathbf{r}'|$, $c^{-2} = \varepsilon \mu$ and $t'$ is the retarded time denoted by $t' = t - R/c$. $\mathbf{n}$ is the inward unit normal vector to the surface. The fields on the boundary $S$ are related to the equivalent surface electric and magnetic current densities ($\mathbf{K}_e$, $\mathbf{M}_s$) and charge densities ($\sigma_s$, $\eta_s$) by

$$\mathbf{n} \times \mathbf{E}_{\text{scat}} = - \mathbf{n} \times \mathbf{E}_{\text{self}} = -\mathbf{M}_s $$

$$\mathbf{n} \times \mathbf{B}_{\text{scat}} = - \mathbf{n} \times \mathbf{B}_{\text{self}} + \mu \mathbf{K}_e $$

$$\mathbf{n} \cdot \mathbf{E}_{\text{scat}} = - \mathbf{n} \cdot \mathbf{E}_{\text{self}} + \sigma / \varepsilon = \sigma_s / \varepsilon $$

$$\mathbf{n} \cdot \mathbf{B}_{\text{scat}} = - \mathbf{n} \cdot \mathbf{B}_{\text{self}} = \eta_s $$

(3)

The equations (1) and (2) can be interpreted as a mathematical expression of the so-called surface equivalence theorem in time domain, which states that the scattered fields in an original problem can be replaced by the fields produced by the surface equivalent current densities and charges.

This approach was named as Scattered-field Time Domain Boundary Element Method (S-TDBEM) [4].

A. Spatial and Temporal Discretizations

In this work, we adopt the magnetic field integral equation (MFIE) in time domain (2) as a basic equation. The surface $S$ is discretized with spatial quadrilateral planar patches as boundary elements and the time axis is divided by constant time step size $\Delta t$. The fields inside a boundary element are spatially expanded into the 2D curl-conforming vector basis function [13], and temporally expanded into the triangular basis function [14] (i.e. linearly-interpolated temporally). The time derivative is approximated by backward finite difference.

The evaluation of the boundary integrals in (2) should be carefully performed. In particular, for the strongly singular kernel terms of self-elements, the Cauchy principal value integration is evaluated, and by virtue of the use of planer patch it can be analytically performed [15]. For the other elements, the integrations can be numerically performed by taking into account the retarded time on the discrete time axis.

After performing this discretization procedure for (2), we finally obtain the following matrix equation:

$$[G_0] \mathbf{b}_t^n = \sum_{k=1}^{n} [G_k] \mathbf{b}_{t-k}^n + \sum_{k=0}^{n} [C_k] \mathbf{b}_{t-k}^n + \sum_{k=0}^{n} [P_k] \mathbf{e}_{t-k}^n, \quad (4)$$

where $\mathbf{b}_t^n$, $\mathbf{b}_{t-k}^n$, and $\mathbf{e}_{t-k}^n$ denote the boundary value vectors which consist of the tangential and normal magnetic field components and the tangential electric field component on the boundary elements at time $t = i \Delta t$ ($i = 0, \cdots, K$), respectively. The coefficient matrices $[G_k]$, $[C_k]$ and $[P_k]$ are determined by the boundary integral of (2), respectively. Then, $\mathbf{b}_t^n$ and $\mathbf{e}_{t-k}^n$ are known boundary value vectors which can be calculated directly from the self-fields in (3). Therefore we finally obtain a system matrix equation as follows:

$$[G_0] \mathbf{b}_t^n = \mathbf{b}_{t-k}^n + \sum_{k=1}^{n} [G_k] \mathbf{b}_{t-k}^n, \quad (5)$$

where $\mathbf{b}_{t-k}^{n-k}$ is the vector resulting from the matrix-vector multiplications of the second and the third terms in the right-hand side of (4) at a time step $\eta$. By solving the reduced matrix equation (5) at each time step, the electric surface current and charge densities induced on the boundary surface of an accelerator structure can be obtained iteratively. The matrix-vector multiplications in term of $\mathbf{b}_t^n$ and $\mathbf{e}_{t-k}^n$ over all time steps should be performed before the system matrix (5) is solved.

Once the boundary values have been obtained over all time steps, the wake fields at any position in the bounded domain can be calculated from (1) and (2).
B. Numerical Stability of System Matrix Equation

The reduced system matrix equation (5) is the starting point of discussion of time domain numerical schemes with the moving window technique in this paper. Note that the matrices $[C_k]$ and $[I_k]$ in the original matrix equation (4) do not contribute to numerical stabilities since the boundary value vectors $b_n$ and $e_n$ multiplied by their matrices are given, and it is not necessary to discuss the matrices $[C_k]$ and $[I_k]$ in terms of the numerical stabilities of S-TDBEM. In order to consider numerical stabilities of (5), we should take into account only a set of the matrices $[G_k]$. Many previous works [16]–[19] indicate that $c \Delta t > h_{\text{max}}$ ($h_{\text{max}}$ is the maximum mesh size) is a stable condition in many practical cases. In fact, this tendency has been numerically validated in the Walker’s eigenvalue analysis [18] for several simple cases. In this choice of time step size, a spherical surface with radius $c \Delta t$ centered at the observation point $r$ contains a lot of neighbor boundary elements, or at least the closest boundary elements. Owing to this situation, the field quantities on a boundary element at the $n$-th time step are not independent of the ones on other adjacent boundary elements at the same time step, and thus the system matrix $[G_0]$ becomes non-diagonal. As $c \Delta t$ becomes larger, the number of boundary elements included in the $c \Delta t$ sphere increases, and therefore the number of non-zero element of $[G_0]$ increases, i.e. the system matrix equation becomes more implicit, and consequently time domain scheme becomes more stable [17]. This choice of $c \Delta t > h_{\text{max}}$ is often called implicit scheme while a choice of $c \Delta t < h_{\text{min}}$ (the minimum mesh size $h_{\text{min}}$) is called explicit scheme. It is well recognized that the explicit scheme is usually very unstable [17], [19]. So, most of time domain boundary element schemes (exactly saying, schemes formulated with temporally local basis function) usually employ the implicit scheme.

We have recently shown that the S-TDBEM formulation [4] is able to achieve long-time numerical stability even with very small time step size. The main reason for the stability is in reforming the scheme from the open scattering to the interior region problems. In Section VI, we will demonstrate that this approach is very stable for practical large-scale problems even in the explicit scheme.

III. MOVING WINDOW TECHNIQUE IN TIME DOMAIN BOUNDARY ELEMENT METHOD

In order to compute the short-range wake fields of a short bunch traversing long accelerator structures at low calculation costs, a moving window technique [12] has been used in Finite Integration Technique (FIT) codes such as TBCI [20], ECHO [21], PBCI [22], and ROCOCO [23]. For the same purpose, we incorporate the concept of this technique into the TDBEM scheme.

It can be understood immediately that implicit schemes (the matrix $[G_0]$ is non-diagonal) cannot be available for the moving window technique in principle because a part of the off-diagonal elements of the matrix $[G_0]$ is corresponding to the contribution of unknown present boundary values outside the moving window, and thus the lack of boundary value information at the tail of moving window arises and it finally results in an unwanted numerical error and its accumulation. Therefore, for a moving window implementation of the TDBEM scheme, we use the explicit S-TDBEM scheme for the system matrix (5), in which the matrix $[G_0]$ is diagonal.

We shall consider the explicit S-TDBEM scheme with moving window technique (S-TDBEM(w)) on a four-dimensional time-space volume which involves a bunch passing through a long multi-cell cavity as shown in Fig. 1. The basic idea of this technique is based on the following facts: (i) no field travels in front of an ultra-relativistic bunch and (ii) the fields inside the moving window with the speed of light synchronized with the bunch are not affected by any fields that happen behind the window. These two points result from causality and the assumption of rigid bunch. From this reason, we can compute only the fields over the space-time volume surrounded by the head and the end of the window (marked in Fig. 1). By taking into account this fact and (5), the S-TDBEM system matrix equation (5) can be reduced for the time domain simulation of boundary value inside the moving window, as shown in Fig. 2. The reduced matrix equation has many small system matrices $[M^n_b]$ determined by the numbers of the boundary value vector elements inside the moving window at each time step $n$. Accordingly, the size of a small system matrix $[M^n_b]$ depends only on the size of moving window, and does not depend on the total size of a structure. Because it is necessary for this scheme to reconstruct all of the small system matrices $[M^n_b]$ at each time step and the matrix $[M^n_b]$ is always diagonal (explicit scheme), storing the matrices $[M^n_b]$ in memory is not needed any more. Therefore, the required memory size of this scheme becomes quite smaller than that of the original TDBEM scheme. This enables us to apply the S-TDBEM(w) for practical accelerator structures as shown in Section VI.
Fig. 3. Parallelization algorithms. In (a), a set of matrix-vector multiplications is executed in each of slave CPUs, and then the resulting vectors from the multiplications are transferred to the master CPU. In (b), the reduced system matrix equation of Fig. 2 is sliced into rows, and a set of sliced multiplication parts is executed in slave CPUs. Therefore only small parts of a vector are communicated between the master CPU and slave CPU in (b). (a) Conventional scheme [7]; (b) proposed scheme for the moving window.

Fig. 4. Contours for wake potential calculation in TDBEM. (i) NCZ method with the contour \( C \) along the boundary cross section of an accelerator structure, (ii) NCZ modified indirect integration (line integral \( L_0 + L_u \)), (iii) 3D indirect integration (line integral \( L_0 + 2D \) Poisson’s equation for pipe cross section area \( A \)).

Fig. 5. Numerical model of the TESLA 9cell cavity.

IV. PARALLELIZATION OF MOVING WINDOW TECHNIQUE

As we mentioned in the previous section, the S-TDBEM(w) scheme is almost free from the problems of memory requirements. However, in the case of very long accelerator structures the calculation time becomes the most significant problem because the number of the system matrices \( [M^n] \) still depends linearly on the total length of an accelerator structure (in realistic accelerator problems the transverse dimension of a structure is usually much smaller compared to the longitudinal size). The number of the time steps increases linearly as well. Hence, the computational effort scales quadratically with the total length. This quadratic scaling law is a main drawback of the developed moving window technique compared to the conventional TDBEM scheme on distributed memory computing environment. A set of the system matrices is almost equally assigned and stored on the distributed memories and each CPU executes the matrix-vector multiplication of (5), and then a set of the calculation result vectors \( [G_0] \) is transferred to the master CPU. After that, the master CPU executes inversion of the system matrix \( [G_0] \) to calculate the newest time step unknown vector \( \mathbf{b} \). Finally, the newest boundary value vector \( \mathbf{b} \) is broadcast to the slave CPUs for the next time step calculation.

For this problem, we consider here a parallelization algorithm suitable for the S-TDBEM(w) scheme.

In the parallelization scheme for the conventional TDBEM in [7], since all of the system matrices are stored in memory and the matrix construction is performed once before time domain calculation, the matrix-vector multiplications in the right-hand side of system matrix equation (5) are most time-consuming and to be parallelized. Fig. 3(a) shows the parallelization of the conventional TDBEM scheme on distributed memory computing environment. A set of the system matrices is almost equally assigned and stored on the distributed memories and each CPU executes the matrix-vector multiplication of (5), and then a set of the calculation result vectors \( [G_0] \) is transferred to the master CPU. After that, the master CPU executes inversion of the system matrix \( [G_0] \) to calculate the newest time step unknown vector \( \mathbf{b} \). Finally, the newest boundary value vector \( \mathbf{b} \) is broadcast to the slave CPUs for the next time step calculation.

By contrast, when the moving window technique is incorporated in the S-TDBEM scheme, since the construction of the matrices \( [M^n] \) is performed at every time step, the calculation of the system matrices \( [M^n] \) is the most time-consuming part in the S-TDBEM scheme and this should be parallelized. In this work the S-TDBEM(w) matrix calculation process is parallelized so that the system matrix equation is sliced into rows. Fig. 3(b) gives a schematic picture of this parallelization algorithm. This approach is also corresponding to longitudinally dividing the moving window. The advantage of the proposed parallelization
algorithm is that the interprocess communication between the master CPU and slave CPUs is much smaller than that of the original TDBEM scheme because only small parts of the calculated vector are transferred to the master PC.

V. W AKE P O TENTIAL C ALCULATION

The wake potential [1], [24] is one of important physical quantities for quantitatively evaluating the wake field effects in the design of an accelerator. In this section we briefly summarize how to compute wake potentials in the framework of TDBEM.

The longitudinal and transverse wake potentials are defined as an normalized integral over the electromagnetic field along a test particle with unit charge following the exciting bunch \( \rho(\mathbf{r}, t) \) with total charge \( Q \) traversing an accelerator structure with the same velocity \( \mathbf{v} \) parallel to the z-axis and the transversal coordinates \( \mathbf{r} \), at a distance \( s \) behind the bunch [24]:

\[
W_L(\mathbf{r}, s) = -\frac{1}{Q} \int_{-\infty}^{\infty} E_z(\mathbf{r}, z, t = (z+s)/v) \, dz, \quad (6)
\]

\[
W_T(\mathbf{r}, s) = \frac{1}{Q} \int_{-\infty}^{\infty} (\mathbf{E}_T + \mathbf{v} \times \mathbf{B})(\mathbf{r}, z, t = (z+s)/v) \, dz. \quad (7)
\]

The transverse wake potential (7) can be obtained from the longitudinal one by applying the Panofsky-Wenzel theorem [25].

To obtain the short-range wake potential of a short bunch in long accelerator structures, direct time domain calculations of wake field are commonly made with the moving window technique and indirect integration methods [8]–[11] are often used in order to dramatically reduce the calculation time in a computer code. In the following, we shall review the implementation of indirect methods for wake potential integration.

For axis-symmetric structures, the infinite integration of wake potential can be replaced by a finite range of integration with the Napoly-Chin-Zotter (NCZ) indirect integration method [11]. Especially, selecting the integration path along the boundary surface of a structure as the path (i) shown in Fig. 4 leads to the simple calculation of the wake potentials from the total electromagnetic fields on the boundary surface, i.e., directly from the boundary values solved [3], [26]. The advantage of this path selection is that it is unnecessary to calculate the fields inside the structure. Although a modification of the NCZ indirect method [21], whose integration path is shown as the path (ii) in Fig. 4, can be also applied for S-TDBEM, additional computation of the inside fields is required. Therefore, the method (i) in Fig. 4 is quite suitable for the S-TDBEM.

For general 3-D structures, the recently developed indirect wake potential integration method [10], [11] can be also applied for the S-TDBEM. The 3-D indirect method needs a direct 1-D integration with finite length and a solution of the 2-D Poisson equation (for details, see [10], [11]) over cross-section of the outgoing beam tube as in Fig. 4. In the framework of TDBEM, the finite direct integration is made by computing the scattered fields along the beam path inside an analytical region using the field integral representations (1) and (2), and the 2-D Poisson equation can be easily solved by a standard 2-D boundary element solver.
VI. NUMERICAL EXAMPLES

A. TESLA 9cell Cavity

Fig. 5 shows a numerical model of the TESLA 9cell cavity [27] as an example of long accelerator structures. The total length of the cavity is about 1 m and the numerical model is assumed to be axisymmetric.

Fig. 6 shows the comparison of wake potentials of the on-axis Gaussian line bunch with RMS length $\sigma = 1$ mm calculated with the S-TDBEM(w) scheme and by a simple square mesh calculation based on a FIT scheme in cylindrical coordinates [20]. In the standard FDTD simulation oscillations are observed while in the S-TDBEM(w) simulation there is no oscillation because of the grid dispersion-free property of the S-TDBEM.

B. TESLA Accelerating Cryomodule

Here we demonstrate an application of the parallelized STDBEM code to very large-scale wake field analysis. As a test example, the TESLA accelerating cryomodule which consists of eight of the TESLA 9cell cavities is simulated as in Fig. 9(a). The total length of the structure is about 11 m, the RMS length of a Gaussian bunch is 1 mm, and the grid resolution is taken to be $\sigma/h = 5$. The number of total time step is about 140000. The simulation is done with 256 CPUs on a supercomputer, the HITACHI SR-11000. The calculation time is about 19 hours.

In this case the high frequency field excited by a short bunch can propagate in the cavity, and therefore the zero grid dispersion property is very important in order to accurately compute wake potentials. As expected, the S-TDBEM(w) calculation shows no oscillation due to the numerical dispersion.
error in Fig. 9(b). We can see excellent agreement between the S-TDBEM (w) and the ECHO [21] codes.

C. Tapered Collimator

Finally we deal with an axially symmetric tapered collimator with geometry parameters \(a = 19 \text{ mm}, b = 1.9 \text{ mm}, d = 0 \text{ mm}, L = 510 \text{ mm}\) as shown in Fig. 10. The geometric parameters are similar to the ones of the collimator that was tested in the SLAC linac [28]. The convergence property of the proposed scheme is tested for this axisymmetric model. Fig. 11 shows the results of loss factor calculated by the S-TDBEM and the code ECHO. The loss factor is defined by

\[
L_{||} = \int_{-\infty}^{\infty} \lambda(s)W_{||}(s) ds,
\]

where \(\lambda(s)\) the shape distribution of a bunch. A good convergence of the S-TDBEM is demonstrated in the comparison of the computed loss factors. A Gaussian bunch with \(\sigma = 4 \text{ mm}\) is used in this simulation. For the mesh resolution \((\sigma/h = 5)\) of almost same accuracy in Fig. 11, the calculation time of our code is about 80 sec with single CPU operation in Intel(R) Core(TM)2 CPU T5500 1.66 GHz/1.67 GHz.

Fig. 12 shows the results of longitudinal wake potential of a short Gaussian bunch \((\sigma = 1.2 \text{ mm})\) traversing an axially symmetric tapered collimator with longitudinally longer dimensions \((a = 19 \text{ mm}, b = 1.9 \text{ mm}, d = 0 \text{ mm}, L = 510 \text{ mm})\). It is found again that the calculation by the S-TDBEM shows faster convergence than the ECHO calculations. We can conclude that for long tapered structures the S-TDBEM works well as a conformal scheme for dispersion-free wake field calculations.

VII. CONCLUSION

An explicit S-TDBEM scheme with the moving window technique (S-TDBEM(w)) has been proposed for dispersion-free wake field simulations of long accelerator structures. The moving window implementation in the framework of TDBEM has been discussed, and the S-TDBEM(w) code has been applied for the TESLA 9cell cavity, the TESLA accelerating cryomodule and the tapered collimators. The numerical examples show good agreement between the numerical results calculated by the presented code and by several FIT codes such as ROCOCO and ECHO.

The simulations by the 2-D S-TDBEM(w) code are done in order to test the developed moving window technique, and only longitudinal monopole wake field calculations are shown in the numerical results. However, this is not a limitation of the developed technique, and the presented method can be applied to transverse dipole and three dimensional wake field calculations as well. A 2.5-D/general 3-D TDBEM code with this moving window technique is indeed being developed for transverse dipole and three dimensional wake field simulations.

In addition, the presented approach is available even if a bunch has curved trajectories when the bunch has very high energies and always moves inside a moving window. That is, the application of this approach is independent of the selection of wake potential integration path. Transient analysis of coherent synchrotron radiation (CSR) shielded by arbitrary 3-D vacuum chambers is another important application of S-TDBEM(w). This application will be presented in near future.

As is mentioned in Section IV, the quadratic scaling law is a main drawback of the developed technique. We are now working in development of an accelerating technique for achieving the linear scaling law of calculation time as in the moving window implementation of FDTD method.

REFERENCES


