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メタデータ	言語: English 出版者: IEEE 公開日: 2016-01-14 キーワード (Ja): キーワード (En): Particle accelerator science, time-domain boundary element method, time-domain microwave simulation 作成者: 川口, 秀樹, ITASAKA, Seiya, WEILAND, Thomas メールアドレス: 所属:
URL	http://hdl.handle.net/10258/3836

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journal or publication title	IEEE transactions on magnetics
volume	51
number	3
page range	7201604-7201604
year	2015-03
URL	http://hdl.handle.net/10258/3836

doi: info:doi/10.1109/TMAG.2014.2361613

4D Space-Time Domain Decomposition Simulation of Particle Accelerator Wake Field Based on 3D Time Domain BEM

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A time domain boundary element method (TDBEM) provides one more possibility of potential numerical schemes for a time domain microwave simulation in addition to the FDTD method. However, it is known that the TDBEM requires very large memory of order of hundred GB. As one of solutions to effective memory reduction, this paper presents four-dimensional (4D) domain decomposition method for the TDBEM. It is shown that 4D domain decomposition method of the TDBEM works well for the effective memory reduction in a particle accelerator wake field analysis.

Index Terms— **particle accelerator science, time domain boundary element method, time domain microwave simulation.**

I. Introduction

A time-domain boundary element method (TDBEM) provides another possibility of potential numerical schemes for time-domain microwave simulations in addition to the FDTD method. The TDBEM has its advantage in coupling problems of microwave and charged particle motion and open/moving boundary problems owing to its feature of surface meshing [1]-[5]. On the other hand, it is known that the TDBEM requires very large storage memory of order of hundred GB and heavy computation cost, and these disadvantages have prevented the TDBEM from being used widely in practical applications.

To improve the problems of the large memory requirement of the TDBEM, the column row storage (CRS) matrix compression was proposed, and indeed, it was shown that effective memory reduction was achieved by the CRS [6]. In addition, the MPI processing scheme which provides suitable memory access for the CRS were also proposed. As one more improvement of memory reduction for the TDBEM, an initial value problem formulation was introduced [7]. It was found that an employment of the initial value problem formulation stabilizes the time domain microwave simulation by the TDBEM and coarser mesh can be used as the result of the stabilization, which also leads to memory reduction. However the employments of the CRS matrix compression and the initial value problem formulation can reduce the required memory only by several factors at most, that is, it is not easy to use the TDBEM for very large scale time domain microwave phenomena, which appear in practical applications.

As a remaining possibility of more efficient memory reduction of the TDBEM, this paper presents a four-dimensional domain decomposition method based on the initial value problem formulation. In addition to the advantage of the stabilization of the time domain simulation, the initial value problem formulation of the TDBEM provides one more benefit of non-zero initial value simulation in the time domain calculation. That is, we can continuously combine the TDBEM simulations to use the field values in the previous sub-domain TDBEM simulation for the initial values in the next time sub-domain. Indeed, it was already shown that this cascade use of the TDBEM on sub-domains was effectively applied to two-dimensional time domain microwave phenomena which are coupling with charged particle beam motion in a particle accelerator (wake field) [8]. Similar techniques were already introduced in both of the FDTD method and the TDBEM as "moving window technique" [9]-[11]. However the moving window technique can be used for a straight beam motion basically. In this paper, the domain decomposition method of the TDBEM is generalized to three-dimensional numerical models, and the presented scheme is applied to a case of curved beam trajectories in the particle accelerator.

II. Initial Value Problem Formulation of 3D TDBEM

In a case of non-zero initial value, the electromagnetic fields (at position **x** and time t) are expressed by the following time domain Kirchhoff's integral equation, which are defined on four-dimensional space-time [7]-[8], (see Fig.1)

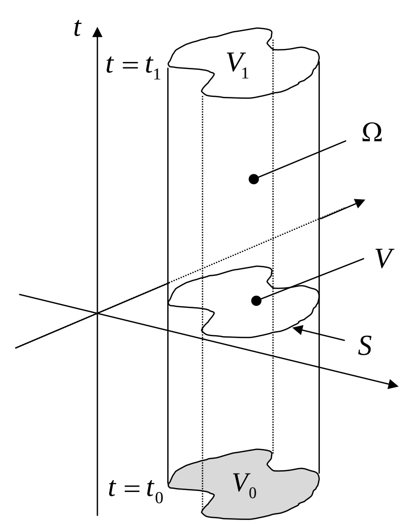

Fig.1 Domain in four dimensional space-time

$$
\begin{aligned}
\mathbf{B}(t,\mathbf{x}) &= \mathbf{B}_{ext}(t,\mathbf{x}) + \frac{1}{4\pi}\int_S \left\{ \frac{\dot{\mathbf{E}}(t',\mathbf{x}')\times\mathbf{n}'}{|\mathbf{x}-\mathbf{x}'|} \right\} dS' \\
&+ \frac{1}{4\pi}\int_S \left\{ \left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \times (\mathbf{n}'\times\mathbf{B}(t',\mathbf{x}')) \right\} dS' \\
&+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) (\mathbf{n}'\cdot\mathbf{B}(t',\mathbf{x}')) \right\} dS' \\
&+ \frac{1}{4\pi}\int_{V_0} \left(\left(\dot{\mathbf{B}}(t',\mathbf{x}') + \frac{\partial \mathbf{B}(t',\mathbf{x}')}{\partial r'} \right) \frac{|\mathbf{x}-\mathbf{x}'|}{c} + \mathbf{B}(t',\mathbf{x}') \right) dV',
\end{aligned} \tag{1}
$$

where $\mathbf{B}_{\rm ext}$ is the externally applied magnetic field, $\mathbf{x}'$ is the position on the boundary surface, $\mathbf{n}'$ is a unit normal vector, and t' is so-called retarded time defined by $t' = t - |\mathbf{x} - \mathbf{x}'|/c$ (c is the velocity of the light in vacuum). The electric field $\mathbf{E}$ is also expressed by a similar integral equation. In particular, the fifth term of the volume integral in (1) implies the contribution from the field values at the initial time (super-surface V_0 in Fig.1). In Figs.2(a) and (b), overview of a time domain matrix equations which are induced from (a) the conventional and (b) the initial value problem formulation TDBEM are shown respectively. It is assumed that the initial boundary values are zero in the conventional TDBEM, and, we need to sum up all of non-zero boundary values $\mathbf{B}_{n-l}$ at the previous time $t - l\Delta t$ (from $l = 1$ to $l = L$, where $\mathbf{B}_{n-L}$ is the first non-zero boundary value) for the calculation of the boundary value $\mathbf{B}_n$ at the present time t. On the other hand, we can start the time domain simulation at any time t_0 if we know all field values in the domain V at the initial time, owing to the existence of the volume integral term for the initial value. (see Fig.2(b))

III. 4D Domain Decomposition of TDBEM Based on Initial Value Problem Formulation

It was shown that the initial value problem formulation of the TDBEM based on (1) can be applied to the domain decomposition method in two-dimensional time domain microwave simulations [8]. That is, we can repeat the calculation of the initial value problem formulation TDBEM to use the boundary values, which are calculated in the previous sub-domain, for the initial boundary values in the next stage sub-domain. (see Fig.3) In particular, this domain decomposition method is effectively used to reduce the memory size of time domain simulations of the microwave which is produced by the moving charged particle beam to

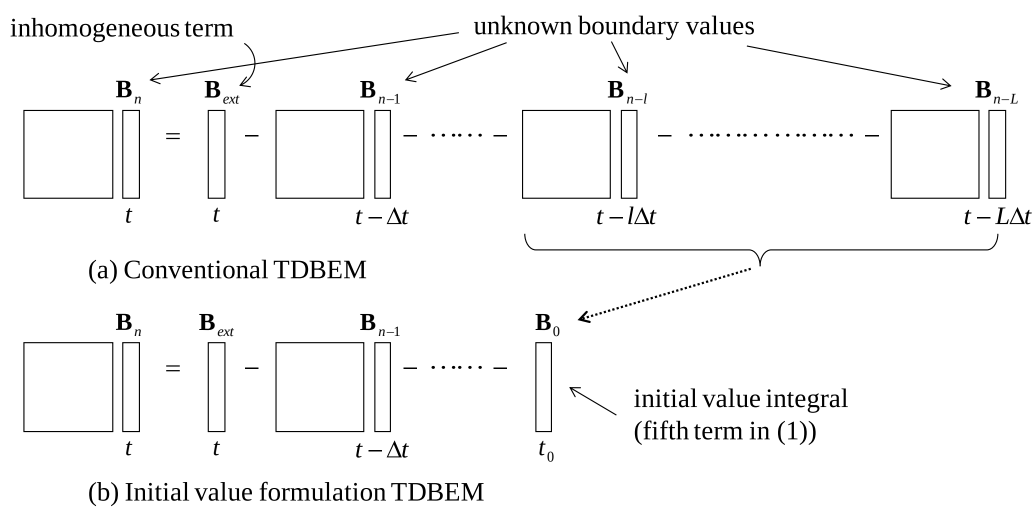

Fig.2 Configuration of matrix equations of (a) conventional and (b) initial value formulation TDBEM

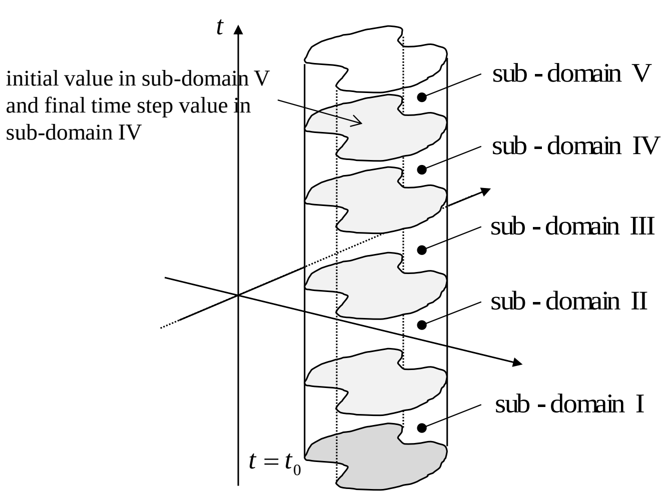

Fig.3 Cascading of sub-domains in 4D domain decomposition method of TDBEM

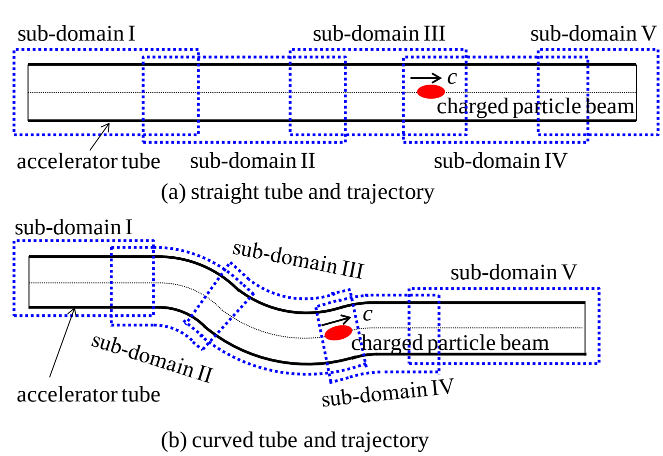

Fig.4 Domain decomposition method in TDBEM synchronizing with charged particle motion

cascade small sub-domains synchronizing with the charged particle beam motion. (Fig.4(a)) We here extend 2D domain decomposition simulation of the TDBEM to 3D numerical models. Then, a straightforward extension of this domain decomposition scheme to three-dimension system leads to a lack of storage memory even if we use supercomputers with 100 GB memory. It is necessary to employ additional efforts of memory reduction such as the CRS scheme [6].

It is known that there exist similar concept schemes called "moving window technique" for both of the FDTD and the TDBEM in numerical accelerator science [9]-[11]. The moving window techniques enable us to simulate extremely long structure microwave problems by cascading much smaller size sub-domains. However, the sub-domains of the moving window techniques are defined along causality line in 4D space-time. This means that use of these techniques is limited to only straight charged beam trajectories with the light velocity in principle. That is, all of conventional domain decomposition methods including Ref.[8] in the time domain microwave simulation schemes can be used only for axisymmetric 2D problems indicated in Fig.4(a), and therefore the presented scheme is a unique solution to solve curved trajectory problems with any velocity (see Fig.4(b)).

IV. Numerical Examples

One of typical applications of 4D domain decomposition method of the TDBEM is transient microwave fields (wake fields) which are produced by relativistic charged particle beams in a bunch compressor of the particle accelerator. Overview of the accelerator tube at the bunch compressor part is indicated in Fig.5(a). When the charged particle beam travels on the center axis of the accelerator tube, the longitudinal component of the surface current is mainly induced, and travels with the original charged particle beam. Although the rotational (or transversal) component of the surface current, which is induced at the curved section, has much smaller amplitude than that of the longitudinal component, it is known that this small component strongly affects to the charged particle beam motion owing to its non-symmetric distribution, and therefore it is very important for analysis of the beam dynamics to understand the time domain behavior of the rotational component of the surface current at the slightly curved section. Then it is easily imagined that the FDTD method is not suitable for such curved boundary and curved beam trajectory owing to its grid discretization, and the TDBEM is a unique solution to the wake field analysis for the bunch compressor. The entire length of the accelerator tube is about 4.5 m and the tube radius is 1cm, on the other hand, the charged beam length is 1.5cm. (see Fig.5(a)) This means that we need to treat very large number of unknowns, which is very difficult task even by high-end supercomputers. We here apply the domain decomposition method of the TDBEM to this problem.

Figure 5(b) indicates *x-z* cross-section of a half numerical model of the entire tube of Fig.5(a) and allocation of sub-domains, which are corresponding to Fig.4(b). The total number of elements of the mesh of the 3D numerical model is 32,652. Owing to three unknowns on each surface patches, two components of the surface current and surface charge densities, the matrix dimension is about 100,000 and the number of the matrices of Fig.1 (denoted by "L") is about 800 in this numerical model. Time domain behaviors of rotational B_m and longitudinal B_l components of the magnetic field (which are corresponding to longitudinal and rotational components of the surface currents, respectively) along the observation line (see Fig.5(a)) on the boundary are shown in Fig.6, which are calculated by 8 MPI parallel processing on the supercomputer, without the domain decomposition method. The rotational component of the surface current is much smaller (by about 100 times) than that of the longitudinal component. In Fig.7, results of the same simulation by the 4D domain decomposition method with two sub-domains are shown. Although small noise appears at the sub-domain

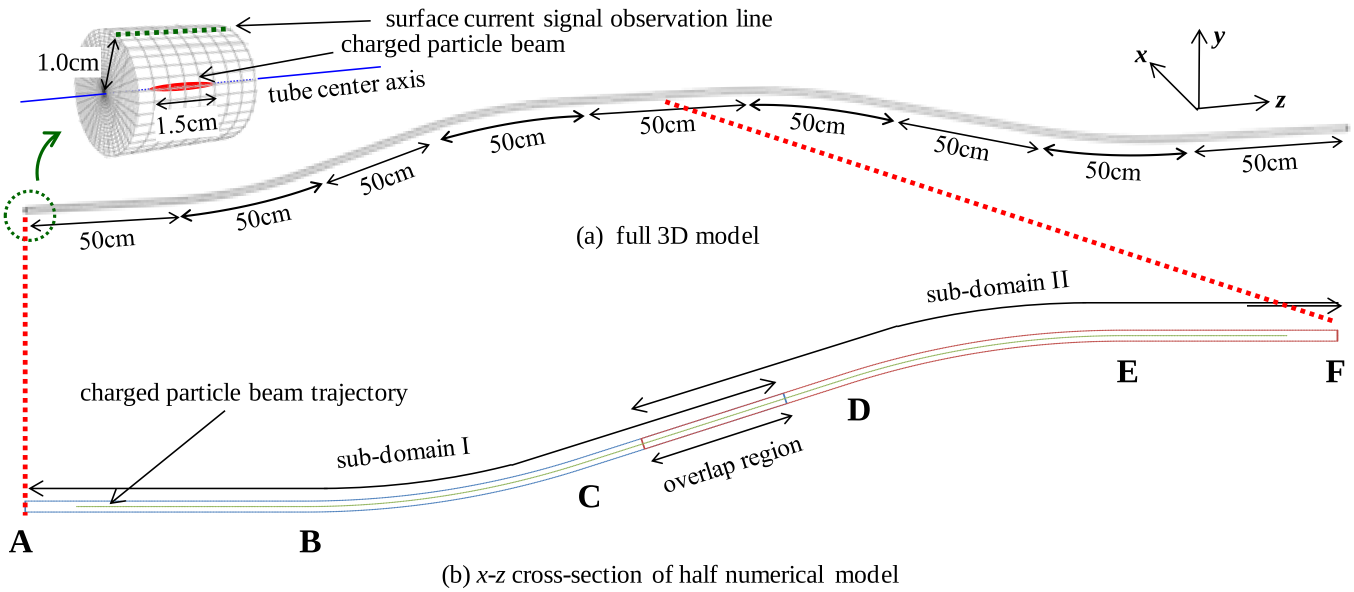

Fig.5 Accelerator tube at bunch compressor of particle accelerator

boundary in Fig.7(b), a good agreement is observed. The required memories for simulations of Fig.6 and Fig.7 were about 168 GB (= 21 GB x 8) and 70 GB, and calculation time were 132 hours (= 16.5 hours x 8) and 18.5 hours, respectively.

V. Summary

In this paper, 4D domain decomposition method of 3D TDBEM based on the initial value problem formulation has been presented. The proposed method is applied to analysis of the wake fields at the bunch compressor part in the particle accelerator. It is shown that the required memory can be effectively reduced compared with that of the conventional TDBEM, and enables us to treat very long accelerator structure which has curved sections by much smaller size memory than those of conventional schemes. In principle, the 4D domain decomposition method of the TDBEM lifts the memory confinement in the wake field analysis for long accelerator structures.

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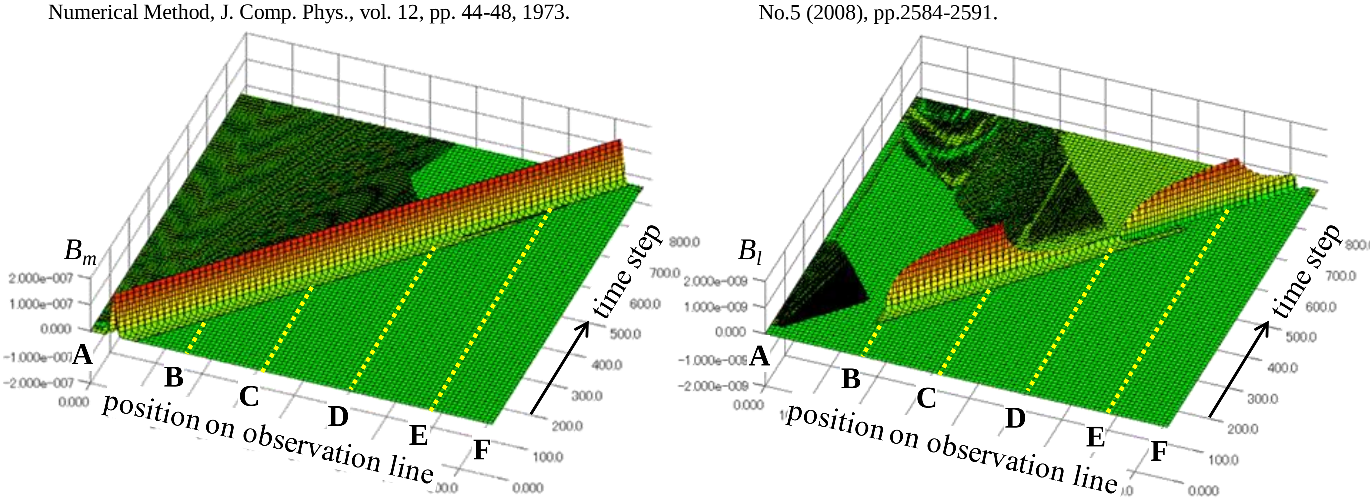
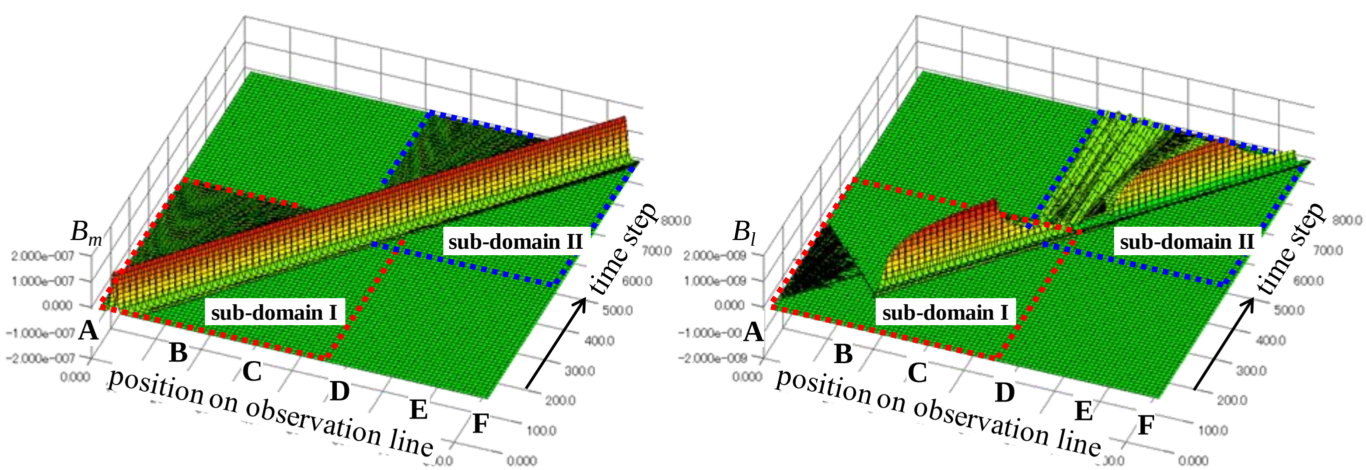


(a) longitudinal component

(b) rotational component

Fig.6 Time domain behavior of surface current along observation line (single domain, simulated by 8 MPI processing)



(a) longitudinal component

(b) rotational component

Fig.7 Time domain behavior of surface current along observation line (simulated by domain decomposition method)