Three-dimensional Time Domain Boundary Element Method with Initial Value Problem Formulation

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***Abstract*— A time domain boundary element method (TDBEM) provides us another possibility for microwave simulation in addition to a time domain finite difference (FDTD) method. The time domain boundary element method has advantages in treatments of open boundary problems, coupling problems with a charged particle motion, etc. On the other hand, the time domain boundary element method has problems of numerical instability in long time range simulation and very large memory requirement. In particular, the numerical instability of the time domain boundary element method mainly comes from interior resonance in an open boundary formulation. In this paper, three-dimensional time domain boundary element method employing an initial value problem formulation is presented to avoid the instability caused by the interior resonance.**

I. Introduction

A time domain boundary element method (TDBEM) provides us another possibility for a microwave simulation in addition to a time domain finite difference (FDTD) method. In particular, the time domain boundary element method has advantages in treatments of open boundary problems, slightly curved boundary shape objects, and coupling problems with a charged particle motion, owing to boundary surface meshing. On the other hand, the time domain boundary element method has problems of numerical instability in long time range simulation and very large memory reqirement. In most cases, the time domain boundary element method is based on an electric and magnetic field integral equations, and the boundary of the domain is assumed to be perfect electric conductor (PEC) [1]-[7]. Then the numerical instability mainly comes from interior resonance owing to an open boundary formulation with the PEC boundary assumption. To avoid the instability caused by the interior resonance in the open boundary formulation, the time domain boundary element method with an initial value problem formulation (IVPF) was presented, and applied to simulations of particle accelerator wake fields [8],[9]. Then, the application of the time domain boundary element method with the initial value problem formulation was limited in two-dimensional axis-symmetric problems owing to the large memory requirement. According to recent remarkable progress of computer memory capacity, three-dimensional time domain boundary element method with the initial value problem formulation is presented in this paper.

II. 3D Time Domain Boundary Element Method with Initial Value Formulation

A standard time domain boundary integral equation method is based on the following time domain electric field integral equation (EFIE) and magnetic field integral equation (MFIE) ;

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

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

$\mathbf{E}_{ext}(t,\mathbf{x})$ and $\mathbf{B}_{ext}(t,\mathbf{x})$ indicate external applied electric and magnetic fields. The integrands in (1) and (2) correspond to surface charge and current densities as follows,

$$\begin{aligned}\mathbf{n}\cdot\mathbf{E} &= \frac{\rho}{\varepsilon}, \\ \mathbf{n}\times\mathbf{B} &= \mu\mathbf{K}, \\ \mathbf{n}\cdot\mathbf{B} &= \rho_M, \\ \mathbf{n}\times\mathbf{E} &= -\mathbf{M},\end{aligned} \tag{3}$$

where ρ, ρ_M, $\mathbf{K}$ and $\mathbf{M}$ are a surface charge density, a magnetic surface charge density, a surface current density and a magnetic surface current density, respectively. ε and μ are dielectric constant and permeability. Eqs.(1) and (2) are kinds of a time domain Kirchihoff's boundary integral equation, that is, those integrands depend on a retarded time t' defined by

$$t' = t - \frac{|\mathbf{x}-\mathbf{x}'|}{c}. \tag{4}$$

When the boundary S is a perfect electric conductor, (2) is reduced to the following very simple form;

$$\mathbf{B}(t,\mathbf{x}) = \mathbf{B}_{ext}(t,\mathbf{x}) + \frac{1}{4\pi}\int_S \left\{ \left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \times \left(\mathbf{n}'\times\mathbf{B}(t',\mathbf{x}')\right) \right\} dS \tag{2)'$$

In the conventional expressions of the EFIE (1) and MFIE (2), it is assumed that all boundary values at an initial time are zero. In general, the time domain boundary integral equations are derived from Green's theorem for a four-dimensional volume region Ω in space time (see Fig.1). Then the surface integral terms in Eqs.(1) and (2) are derived from the integration only on the lateral hyper surface V_s in Fig.1, which is a direct product of two-dimensional surface S of a scatterer and time t. Accordingly, the most generalized formula should include the contribution from the bottom hyper surface V_0 as well, which is pure three-dimensional volume integration at the initial time (Any fields on the top hyper surface V_1 can not contribute to the fields inside the considered space-time domain Ω owing to causality) Then the generalized time domain EFIE and MFIE are obtained as follows [8],[9];

$$\begin{aligned}\mathbf{E}(t,\mathbf{x}) &= \mathbf{E}_{ext}(t,\mathbf{x}) \\ &+ \frac{1}{4\pi}\int_S \left\{ \frac{\mathbf{n}'\times\dot{\mathbf{B}}(t',\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right\} dS \\ &+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \left(\mathbf{E}(t',\mathbf{x}')\cdot\mathbf{n}'\right) \right\} dS \\ &+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \times \left(\mathbf{E}(t',\mathbf{x}')\times\mathbf{n}'\right) \right\} dS \\ &+ \frac{1}{4\pi}\int_{V_0} \left(\left(\dot{\mathbf{E}}(t',\mathbf{x}') + \frac{\partial \mathbf{E}(t',\mathbf{x}')}{\partial r'} \right) \frac{|\mathbf{x}-\mathbf{x}'|}{c} + \mathbf{E}(t',\mathbf{x}') \right) dV',\end{aligned} \tag{5}$$

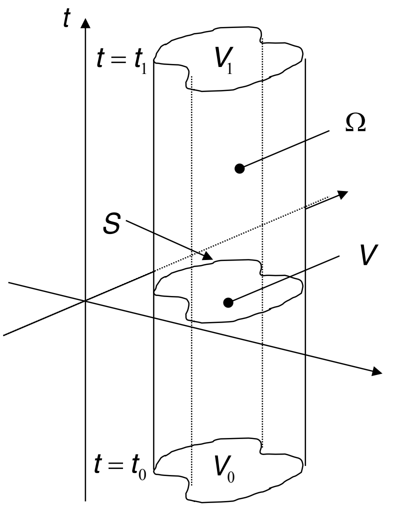

Fig. 1 Four-dimensional space-time region

$$\begin{aligned}\mathbf{B}(t,\mathbf{x}) &= \mathbf{B}_{ext}(t,\mathbf{x}) \\ &+ \frac{1}{4\pi}\int_S \left\{ \left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \times \left(\mathbf{n}'\times\mathbf{B}(t',\mathbf{x}')\right) \right\} dS \\ &+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \left(\mathbf{n}'\cdot\mathbf{B}(t',\mathbf{x}')\right) \right\} dS \\ &+ \frac{1}{4\pi}\int_S \left\{ \frac{\dot{\mathbf{E}}(t',\mathbf{x}')\times\mathbf{n}'}{|\mathbf{x}-\mathbf{x}'|} \right\} dS \\ &+ \frac{1}{4\pi}\int_{V_0} \left(\left(\dot{\mathbf{B}}(t',\mathbf{x}') + \frac{\partial \mathbf{B}(t',\mathbf{x}')}{\partial r'} \right) \frac{|\mathbf{x}-\mathbf{x}'|}{c} + \mathbf{B}(t',\mathbf{x}') \right) dV',\end{aligned} \tag{6}$$

The fifth terms of Eq.(5) and (6) indicate contributions from the bottom hyper surface V_0. To employ Eqs. (5) and (6), the time domain numerical simulation based on the boundary integral equation is free from the confinement of the zero initial value assumption, which is assumed in the conventional time domain integral equation method.

To discretise Eqs.(5) and (6) in space-time according to the formulation of the boundary element method, we can obtain a matrix equation with respect to the surface charge and current densities of the time domain boundary element method for simulation of microwave phenomena taking into account the initial values.

III. 2D Axis-symmetric Problems

If all domain boundaries are the perfect electric conductors, unknown variables are only $\mathbf{n}\cdot\mathbf{E}$ and $\mathbf{n}\times\mathbf{B}$ of (3) owing to the boundary condition. To remove the assumption of the perfect electric conductor, we need to consider all kinds of unknowns of (3) on the domain boundary, and calculation size becomes larger than that of the perfect electric conductor boundary. When the electromagnetic fields are axis-symmetric, a tangential component of the magnetic field oriented to rotational direction B_s, a normal component of the electric field E_n and a tangential component of the electric field perpendicular to rotational direction E_t exist, and the calculation is reduced to reasonable size compared with full three-dimensional problems. Figure 2 indicates a configuration of the system matrix equation of the time domain boundary element method with the initial value problem formulation in the axis-symmetric problems. Owing to retarded time property of (4), k-th time step unknowns B_s^k, $E_n{}^k$, $E_t{}^k$ are calculated using convolutions of the previous time unknowns B_s^{k-l}, $E_n{}^{k-l}$, $E_t{}^{k-l}$. The first term of the right-hand side in Fig.2 is an inhomogeneous term, which consists of the first and fifth terms of Eqs.(5) and (6).

$$\begin{bmatrix} G_{ss}^0 & \mathbf{0} & G_{st}^0 \\ G_{ns}^0 & G_{nn}^0 & G_{nt}^0 \\ G_{ts}^0 & G_{tn}^0 & G_{tt}^0 \end{bmatrix} \begin{bmatrix} B_s^k \\ E_n^k \\ E_t^k \end{bmatrix} = \begin{bmatrix} B_{ext\,s}^k \\ E_{ext\,n}^k \\ E_{ext\,t}^k \end{bmatrix} - \sum_{l=1}^{L} \left(\begin{bmatrix} G_{ss}^l & \mathbf{0} & G_{st}^l \\ G_{ns}^l & G_{nn}^l & G_{nt}^l \\ G_{ts}^l & G_{tn}^l & G_{tt}^l \end{bmatrix} \begin{bmatrix} B_s^{k-l} \\ E_n^{k-l} \\ E_t^{k-l} \end{bmatrix} \right)$$

Fig. 2 System matrix equation of 2D TDBEM with IVPF

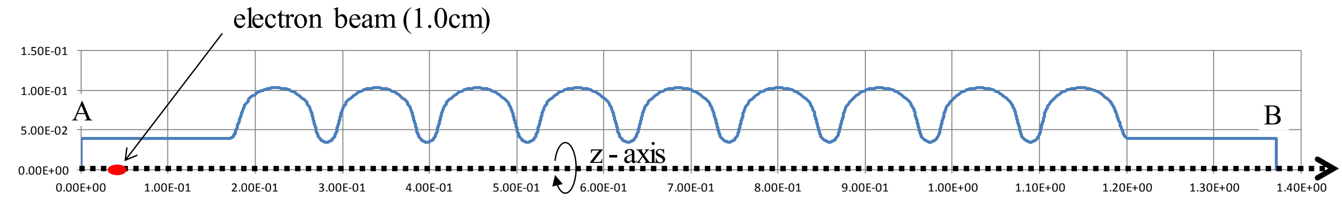

Fig. 3 Cross-section shape of axis-symmetric accelerator cavity

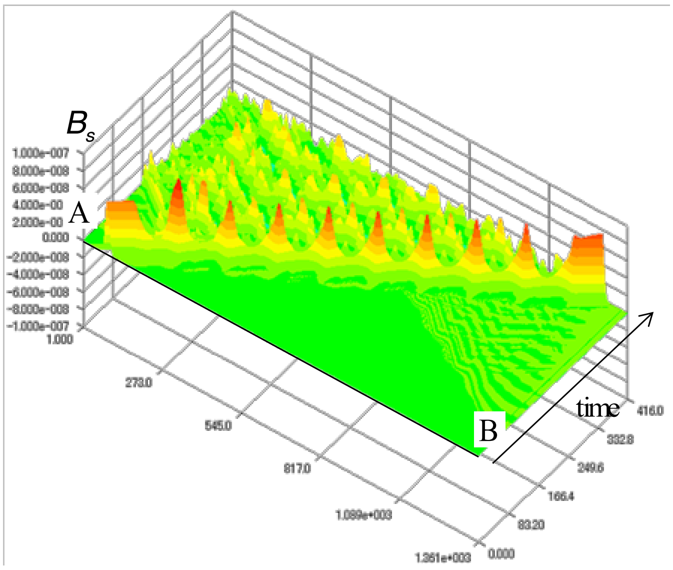

Fig. 4 Time domain behavior of induced surface current

In Fig.3, a cross-section of a numerical example of a particle accelerator cavity, which has axis-symmetric structure, is shown. It is assumed that an electron beam with 1cm length travels on the z-axis from the left-hand side to the right with the velocity of the light c. A simulation result of the time domain behavior of B_s on the cross-section boundary indicated by "A-B" in Fig.3, which corresponds to the induced surface current, is shown in Fig.4. When the electron beam travels on the upstream uniform part, uniform surface current is induced and moves to the downstream with the electron beam. On the other hand, the surface current distribution is disturbed soon after the electron beam arrives at the discontinuous cross section part. It is found that stable simulation is obtained although domain boundary is complicated shape and the simulation is carried out for relatively long time range. In this simulation, the number of meshes on the cross-section line of Fig.3 is 1400, therefore, each sub-matrix size in Fig.2 is 1400 x 1400, and the required memory was 50 GB.

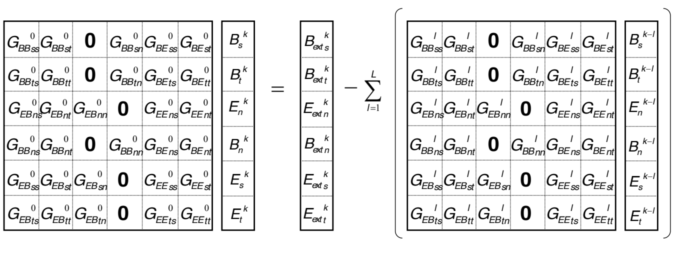

Fig. 5 System matrix equation of 3D TDBEM with IVPF

IV. Full 3D Problems

For full three-dimensional simulation by the time domain boundary element method with the initial value problem formulation, we need to consider all kinds of surface charges and currents of (3). The configuration of the system matrix equation is indicated in Fig.5. The system matrix structure is complicated. In addition, size of each sub matrix is much larger than those of Fig.2, since the number of surface meshes is itself very large. Accordingly, it is predicted that much larger memory will be required in three-dimension time domain boundary element method with the initial value problem formulation than that of conventional formulation.

Figures 6(a) and (b) indicate numerical models of an electron beam motion inside a slightly curved accelerator tube. The numerical model of Fig.6(a) is for the conventional formulation (2)' and has an open boundary structure with torus topology. On the other hand, Fig.6(b) is for the initial value problem formulation and has a closed boundary structure. In the initial value problem formulation, the electron beam should be located inside the closed region always, therefore the numerical model is enlarged compared with Fig.6(a) at the upstream and downstream most. In the both models, the tube radius is 1cm. At the curved section, the curvature radius is 1.6 m and the arc angle is 10 degree. The length of the electron beam with Gaussian line distribution is assumed to be 1.5cm. In this case, there exists a rotational component of the induced surface current in addition to a longitudinal direction owing to three-dimensional property of the fields. Simulation results of the longitudinal component of the induced surface current for both the conventional and initial value problem formulation were almost same each others, and omitted here. In Fig.7, time domain behavior of the rotational component of the induced surface current on the observation line (see Fig.6) are indicated. Fig.7(a) and (b) are for the conventional and initial value problem formulations, respectively. In particular, it is found that the initial value problem formulation gives us much more stable simulation than that of the conventional formulation owing to the closed numerical model structure. Accordingly, it is possible to use coarser meshes than those of the conventional formulation owing to the improvement of the stability. The number of division for the rotational direction was 100 in Fig.6(a) and 20 in Fig.6(b). Then, required memory in the initial value problem formulation was 85GB, which was much smaller than that of the conventional formulation (350GB), although the size of system matrix equation of Fig.5 is much larger than that of the conventional formulation (see Eq.(2)').

V. Conclusion

In this paper, three-dimensional time domain boundary element method with the initial value problem formulation has been presented. It is shown that the initial value problem formulation gives us more stable simulation of microwave phenomena and smaller required memory compared with the conventional formulation. It was pointed out that the time domain boundary element method with the initial value problem formulation can be applied to a space-time domain decomposition method, and required memory can be much more effectively reduced [8],[9]. The 3D TDBEM with the IVPF employing the space-time domain decomposition method will be also presented in near future.

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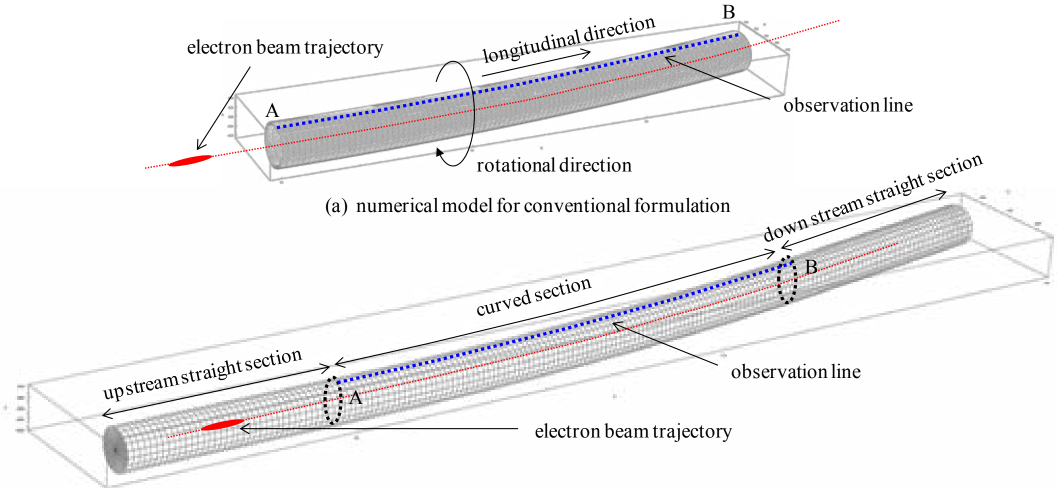
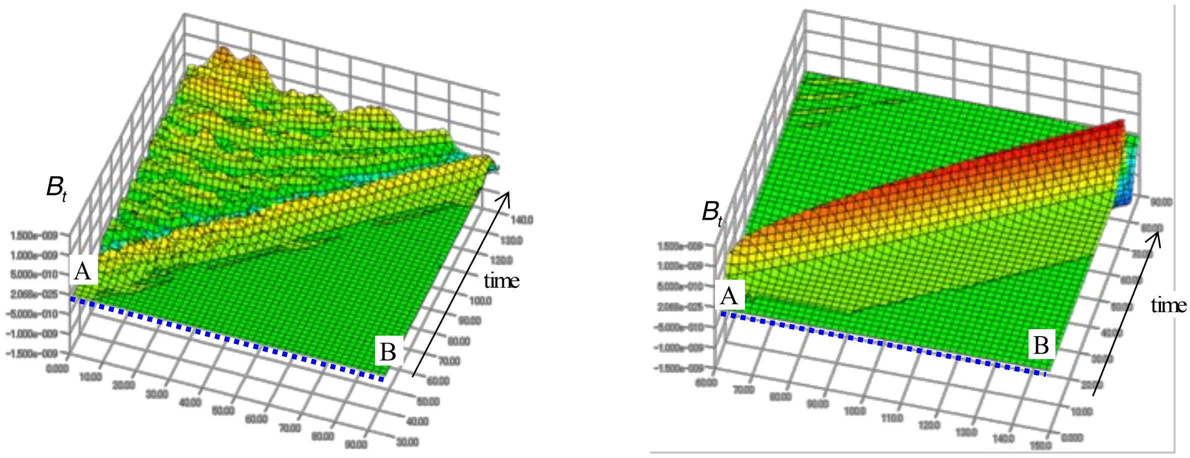


(a) numerical model for conventional formulation

(b) numerical model for initial value problem formulation

Fig. 6 Numerical models of electron beam motion in curved accelerator tube



(a) conventional formulation

(b) initial value problem formulation

Fig. 7 Time domain behavior of induced surface current (rotational direction)