MPI PARALLEL COMPUTATION OF WAKE FIELDS BY USING TIME DOMAIN BOUNDARY ELEMENT METHOD

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Abstract

This paper presents particle accelerator wake fields simulations by using the Time Domain Boundary Element Method (TDBEM) on a system for the MPI parallel computation. It is shown that the parallel scheme of the TDBEM effectively function for performance enhancement in the case of axis-symmetric fields. It is also shown that, in the numerical calculation of wake fields for the TESLA cavity, the TDBEM shows good agreements with that of the FIT code.

INTRODUCTION

Computation of wake field in particle accelerators has been performed in both analytical and numerical methods. Analytical methods can treat only structures with simple geometry, such as a pillbox cavity [1] and a spherical cavity [2]. Numerical methods are able to calculate wake fields excited in more practical and complicated structures. So far, the Finite Integration Technique (FIT) [3] has been widely used as the numerical method for the wake field computation. For this, the authors have been working in development of the Time Domain Boundary Element Method (TDBEM) [4] as one more possibility for the wake field numerical computation. The TDBEM is based on Kirchhoff's boundary integral formulation of electric and magnetic fields. Therefore, the wake fields and charged particle self-fields can be clearly split each other and the wake fields are expressed by the surface current and charge excited by charged particles bunches in the TDBEM formulation, and then it is easy to treat curved boundary shapes. These features are suitable for coupled of charged analysis particles dynamics and electromagnetic fields. On the other hand, the TDBEM has serious problems of heavy calculation cost, large required memory, and numerical instabilities. These problems prevent from applications of the TDBEM to practical problems. For example, the TDBEM can be applied for 3D electromagnetic scattering problems of less than 100 mesh numerical models at most even if it is performed on platform of supercomputers.

In this paper, the authors present improvement of the TDBEM from view points of computation cost, required memory and numerical instability by using MPI parallel computation platform. Simulation results are compared with that of the ECHO code [6], which is based on a conformable scheme to the FIT.

WAKE FIELD ANALYSIS IN TDBEM

The TDBEM is based on the following Kirchhoff's boundary integral formulation of electric and magnetic fields in time domain:

$$\mathbf{E}(t,\mathbf{r}) = \mathbf{E}_{ext.}(t,\mathbf{r}) - \frac{1}{4\pi} \int_{S} \frac{\dot{\mathbf{B}}_{t}(t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dS' \qquad (1)$$
$$- \frac{1}{4\pi} \int_{S} \left[\frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}|^{3}} + \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^{2}} \frac{\partial}{c\partial t} \right] E_{n}(t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}, \mathbf{r}') dS',$$
$$\mathbf{B}(t,\mathbf{r}) = \mathbf{B}_{ext.}(t,\mathbf{r})$$
$$- \frac{1}{4\pi} \int_{S} \left[\frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}|^{3}} + \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^{2}} \frac{\partial}{c\partial t} \right] \times \mathbf{B}_{t}(t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}, \mathbf{r}') dS', \qquad (2)$$

where **r** is the observation point, **r'** the point on the boundary elements, and $t' = t - |\mathbf{r} - \mathbf{r'}|/c$ the retarded time. The integrand \mathbf{B}_t denotes the tangential component of the magnetic field, E_n the normal component of the electric field on the boundary *S*, and \mathbf{E}_{ext} and \mathbf{B}_{ext} denote the external electric and magnetic fields, respectively.

In time domain numerical simulation based on (1) and (2), the time axis is divided into constant segments Δt and the time derivative is approximated by backward finite difference. Numerical models are discretized by planner rectangular meshes. The discretization of (1) or/and (2) and application of electric perfect conductor boundary condition yield the following system matrix equation, which has multi-matrix structure of Fig.1:

$$[M_0][B_n] = [B_{ext}] - \sum_{l=1}^{L} [M_l][B_{n-l}], \qquad (3)$$

where $[B_l]$ is unknown vector spatially discretized at time $t = l\Delta t$, and $[M_l]$ denotes the coefficient matrix determined by the boundary integral (2). Then the total number of the coefficient matrices *L* is finite and it depends on the size of individual numerical models. That is, in the time marching simulation, the unknown boundary values B_t are iteratively calculated by using past values $B_{t-\Delta t}$, \cdots , $B_{t-n\Delta t}$. Once the boundary values are calculated, the electric and magnetic fields in the analytical region can be obtained from (1) and (2).



Fig.1: Structure of system matrix equation of TDBEM.

When the TDBEM is applied to wake field analysis, the boundary integral terms in (1) and (2) can be interpreted as wake fields excited in accelerating structures. Therefore, the fields \mathbf{E}_{total} , \mathbf{B}_{total} can be analytically split into the particle bunch self-fields \mathbf{E}_{self} , \mathbf{B}_{self} and wake fields \mathbf{E}_{wake} , \mathbf{B}_{wake} as follows:

$$\mathbf{E}_{\text{total}} = \mathbf{E}_{\text{self}} + \mathbf{E}_{\text{wake}}, \quad \mathbf{B}_{\text{total}} = \mathbf{B}_{\text{self}} + \mathbf{B}_{\text{wake}}$$
(4)

PARALLEL COMPUTATION SCHEME OF TDBEM

The 3D TDBEM simulation requires, in general, quite heavy calculation cost and large storage memory, and it is almost impossible to be applied to practical problems even if it is performed on platform of supercomputers. So we assume here axis-symmetry for the numerical models. Although the assumption of axis-symmetry indeed reduces the number of available practical applications, there still remain many useful applications under the axissymmetry assumption. Even in the case of the axissymmetric fields, the matrix equation (3) still requires us large storage memory because of the multi-matrix structures of the TDBEM scheme. However, parallel computations show us possibility of remarkable performance improvement under this assumption. In the case of the axis-symmetric system, individual TDBEM matrices $[M_l]$ can be stored in a single PC memory. Then if we store the individual TDBEM matrices $[M_i]$ in each PC in the parallel computation platform system (see Fig.2), communication between the PCs is only vector values of $[M_1]$ multiplied by $[B_1]$ which is quite small traffic comparing with whole process, and therefore high performance scalability can be achieved [4]. And, in addition to the performance improvement, total storage memory size can be increased without serious performance degradation.



Fig.2: Parallel computation and memory distribution.

IMPROVEMENT OF INSTABILITY AND ACCURACY OF TDBEM

Problems of instabilities and accuracy in the time domain boundary integral equation method have been discussed mainly in antenna and microwave engineering fields for a long time since 1970s and several effective improvement methods for the instabilities and accuracy were presented.

In the TDBEM, some of such improvement methods are imported. It is found that Rao's smoothing scheme [6] and Rynne's averaging scheme [7] are especially effective for improvement of accuracy of surface charge density calculation and long range instability, and indeed these schemes are invoked in the TDBEM.

NUMERICAL RESULTS

At the final part of this paper, we show some numerical example of wake field simulations by the TDBEM which are performed on a MPI parallel computation platform. The figure 3 shows a numerical model of a simple pillbox cavity (d = 0.6 mm, R = 6.0 mm, L = 12.0 mm, w = 2.4 mm, $\sigma=3$ mm), and comparison of wake potentials for this model which are calculated by analytical formula, the FIT and the TDBEM are shown in Fig.4. In Fig.5, time domain signals of E_z component in inner region are shown.

One more numerical example is the TESLA cavity shape (see Fig.6). In Fig.7, short range longitudinal wake potentials for RMS = 6mm are shown for several mesh sizes to confirm numerical convergence. And comparison of long range longitudinal wake potentials calculated by the TDBEM and the ECHO code [5] is shown for RMS=3mm bunch size (Fig.8a) and RMS=6mm bunch size (Fig.8b). We can find good agreements in each numerical result.

SUMMARY

This paper has presented the particle accelerator wake field simulation by the TDBEM on the MPI parallel computation platform. Improvement methods for computation cost, required memory, numerical instabilities in the TDBEM are shown. Numerical examples by the TDBEM for the pill-box cavity and the TESLA cavity shape shows good agreements with that of the FIT.

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Fig.5: Time signal of z-component of electric field.



Fig.6: Numerical model of TESLA cavity.



Fig.7: Convergence of the TDBEM simulation.



Fig.8: Comparison of longitudinal wake potentials for TESLA cavity and bunch with $\sigma = (a)$ 3mm, (b) 6mm.