Numerical Modeling and Computation of Radio Frequency Devices

Dissertation

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Abstract

The numerical simulation of radio frequency devices is addressed in this dissertation, including the methods in frequency domain and time domain.

In frequency domain, an embedded domain decomposition method (DDM) is presented herein for solving electromagnetic (EM) problems with complex geometries. In the method, the original computational domain is decomposed into a background subdomain and multiple embedded subdomains. The subdomain problems are easier to solve than the original problem. Furthermore, the shapes of the subdomains can be geometrically non-conformal, and the discretizations in the subdomains are allowed to be completely independent. Information exchange between the subdomains are addressed with respect to four ingredients: field continuity, material difference, perfect electrical conductor (PEC), and port. Field continuity on the subdomain boundaries is weakly enforced by employing Robin transmission condition. Modified volume sources are introduced to account for the material difference between the subdomains. For PEC and port, surface currents on them in the embedded subdomains are impressed into the background subdomain in a proper way.

The numerical properties of the proposed DDM, such as accuracy and convergence, are well demonstrated through several examples. Furthermore, we illustrate its usefulness and flexibility via several engineering problems of practical interest,
including the applications in electromagnetic compatibility (EMC), antenna design, and integrated circuit (IC) analysis.

With the benefits of embedded meshes, the modification of one subdomain will hardly affect the discretization and matrix computation of another subdomain. As a consequence, the introduced method offers a high degree of flexibility in modeling and simulation, and facilitates moving/replacing/adding objects in a background problem straightforwardly. Such feature and flexibility would be desirable in practical and industrial applications, especially for situations where a variety of multiscale components need to be analyzed or optimized.

In time domain, we develop an approach to integrate the discontinuous Galerkin time-domain method (DGTD) with nonlinear circuit simulation. The simulation problem of mixed EM structure and circuit devices is decomposed into an EM subsystem and a circuit subsystem. The EM part is solved with the interior penalty DGTD approach, while simulation program with integrated circuit emphasis (SPICE) and input/output buffer information specification (IBIS) models are investigated for circuit simulation. The two subsystems are coupled through circuit ports based on the concept of impedance surface. A self-consistent scheme is proposed to establish the coupling within a convergent looping form. Finally, the accuracy and robustness of the developed program are demonstrated through the treatments of practical electronic systems with SPICE and IBIS circuits.
To my parents
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Chapter 1: Introduction

In antenna and microwave engineering, computational electromagnetics (EM) plays a prominent role for accurate prediction of the electric performance of radio frequency devices. Many radio frequency devices such as antennas can be considered as linear. To simulate such devices, we usually employ frequency-domain methods. In this work, we propose an embedded domain decomposition method (DDM) for numerical simulation. When a device contains nonlinear circuits, such as diodes and transistors, time domain methods are preferred to capture the nonlinear phenomena accurately. Herein, we present an EM-circuit co-simulation method based on the discontinuous Galerkin time domain (DGTD) method.

1.1 Background in Frequency Domain Simulation

A critical prerequisite for numerical EM simulations is the reliable mesh generation. With the ever growing complexity in the geometries of modern devices, constructing a single-domain mesh of good quality accordingly is becoming an increasingly time-consuming and painful task. Even if such mesh can be constructed, the associated simulation would usually require a prohibitive amount of memory and a long computation time.
The nonoverlapping DDM [1–19] has received considerable attention, as a powerful preconditioner for the vector finite element method (FEM) [20–22]. It starts by dividing the original problem domain into several smaller and disjoint subdomains. Each subdomain can be meshed independently and solved locally while the communication between subdomains is achieved by employing Robin-type or second-order transmission conditions (TCs) iteratively. The inherent divide-and-conquer strategy of nonoverlapping DDM makes it very appealing for simulating large and complex problems such as antenna array [8,11,13], electromagnetic band gap (EBG) [9], multilayer printed circuit board (PCB) [17], etc.

Moreover, a practical problem probably comprises a variety of multiscale objects, such as a cell phone containing multiple transmitting/receiving antennas within it. In design and optimization processes, we often need to adjust the positions, geometric parameters, and material properties of these components. Consequently, repetitive simulations are frequently required. In the conventional FEM, however, a simple geometrical modification will break the global conformity of the mesh, resulting in object re-meshing and system matrix re-computation. Since we need to try many possible parameters in the design or analysis process, a large amount of time could be wasted on the associated repetitive modelings and discretizations. Even in existing nonoverlapping DDM techniques, although nonconformal surface meshes are allowed on the touching interfaces between the adjacent subdomains, the shapes of the touching interfaces are still constrained to be geometrically conformal, as required by the TCs on the touching interfaces. This limitation becomes inconvenient when we need to perform parameter studies on geometries, because re-modelings and re-meshings are still unavoidable if we want to change the boundary shape of a subdomain or
add/replace another component. All these complications impose great challenges on the efficient modeling and design of complicated EM systems.

An attractive technique for repetitive modeling and simulation is to separate the geometrical details of interest and the rest geometries in a problem. The key idea is to embed a subdomain into a background subdomain by using overlapping/embedded meshes, so that the modification of the embedded subdomain does not affect the geometries and discretization in the background subdomain. Such methods have emerged in the applied mathematics and fluid dynamics communities [23–26] in the past several years. For example, in the Chimera overset-grid method [25], complex geometries are divided into a system of geometrically simple composite grids, and an interface scheme is employed to facilitate communication between adjacent grids. In particular, this method has been used widely to numerically simulate systems of conservation laws in fluid dynamics. In reference [26], an overset-grid-based numerical algorithm was developed to solve unsteady, incompressible Navier-Stokes equations for complex, massively separated, three-dimensional flows.

Similar work does exist on the applications of overlapping meshes in electromagnetics. It is worthwhile to mention the insightful overlapping DDM presented in [27] for the simulation of electrically small features. The method introduced overlapping meshes between the subdomains and was achieved by directly enforcing the equivalence of vector wave equations in the tetrahedrons within the overlapping region. Unfortunately, the work did not validate the developed algorithm on cases with possible material difference between the subdomains, which should be an essential functionality of the proposed method. Another problem is that the method needs auxiliary
meshes to represent zero electric fields in a PEC volume, making the implementation inconvenient.

There are several other methods also aiming at improving the efficiency of repeated simulations and parametric optimizations. One example is the mesh deformation/morphing technique [28–31]. In this approach, an existing mesh can be smoothly transformed to conform the geometrical modifications caused by design variations. However, a linear system of equations requires to be solved to update the mesh and the complexity depends on the number of vertices in the mesh. For complex geometries, the cost of the method would be high. Furthermore, mesh morphing is carried out according to the changes of the existing geometries. It is not guaranteed to work when a completely new object is introduced into the computational domain. Another attractive method is the isogeometric analysis [32–35], which employ geometrical information to define basis functions, thereby straightforwardly connecting the numerical simulation with computer aided design (CAD) tools. However, to the best of the authors’ knowledge, the applications of the method in electromagnetics have been limited to two-dimensional problems or simple geometries due to the complexity in establishing curl-conforming spline spaces. Moreover, most CAD tools use connected surface elements to represent volume objects. Hence, trivariate splines may need to be constructed manually for the interior regions.

In this dissertation, a novel embedded DDM is introduced for EM modeling and design. We shall develop the method by addressing the geometrical and material differences between the subdomains. Firstly, a computational domain is decomposed into simpler background and embedded subdomains. Afterwards, each subdomain
is meshed independently and solved with FEM separately. The key step is the identification and appropriate formulation of four types of important information to be exchanged among the subdomains: field continuity at the boundary, material difference, PEC, and port. All the information will be calculated and imposed onto the subdomains iteratively until the overall solution converges to a desired accuracy.

The proposed method allows for completely nonconformal subdomains. Thus, each subdomain can choose mesh size appropriate for its local geometrical details. Furthermore, the proposed embedded DDM facilitates adding and/or replacing objects in the problem domain in a straightforward manner.

1.2 Background in Time Domain Simulation

The past several decades have witnessed a continuing downscaling of integrated circuit (IC) feature sizes. To take advantage of this advancement, IC designers are integrating more components and functional blocks into a single electronic system in the forms of various 3-D stacking technologies. The ever increasing device densities and complexities, together with higher clock frequencies, impose growing challenges in the efficient prediction of signal integrity (SI) in IC designs and analyses.

Equivalent circuit simulation [36–38] plays an essential role in IC engineering because it runs fast and is easy to use. However, electromagnetic field effects in high frequencies, such as skin effect and signal crosstalk, cannot be accurately captured by pure circuit modeling. This is especially true when 3-D device packaging and dispersive materials are used in circuit designs. In contrast, full wave simulation inherently includes high frequency phenomena such as EM coupling, radiation, and
attenuation, thus giving a better description of the SI performance of a complicated IC design.

On the other hand, semiconductor chips or devices contain complicated linear or nonlinear components, and play crucial roles in the proper functioning of circuit designs. Therefore, mixed electromagnetic and circuit co-simulation has become imperative in the design process of PCB products.

Over the past decades, considerable efforts have been made to time-domain EM-circuit co-simulation [39–51]. Among them, the finite-difference time-domain (FDTD) method [39–42] and the finite-element time-domain (FETD) method [43–46] have been well studied and documented. FDTD [52] is extensively used because of its simplicity and efficiency. However, it suffers from numerical dispersion errors and low order approximation of complicated objects. By contrast, FETD [53] offers the robust and accurate modeling of complex geometries, and therefore is preferable when sophisticated 3-D systems need to be solved. Nevertheless, FETD requires a globally conformal mesh and solving a global system matrix equation at each time iteration. For large-scale problems, the computation tends to be expensive and the flexibility is limited by the conformal discretization.

The DGTD method [47–51,54–58] offers an appealing alternative for solving time-domain Maxwell’s equations. It can well address elements of various shapes, non-conformal meshes, and non-uniform degrees of approximation. Allowing for discontinuity in the discrete trial and test spaces, DGTD can provide a substantial amount of flexibility in problem discretization. Furthermore, information exchange is required only between adjacent elements regardless of approximation orders and shapes. This
feature makes it highly suitable and efficient for parallelization [59]. Therefore, the application of DGTD in EM and circuit co-simulation is very promising.

Another important factor in EM-circuit co-analysis is the choice of circuit simulation. In [45], FETD was employed for EM simulation and modified nodal analysis (MNA) simulation was used to build the circuit solver. Similarly, in [49] and [50], the authors chose DGTD for EM simulation while adopted MNA to represent the circuit. In these works, the equivalent circuit representations of metal-semiconductor field-effect transistor (MESFET), for example, were built inside the EM-MNA code and the MNA equations were coupled directly within the FETD/DGTD equations to set up co-simulation. However, it is well known that a general circuit simulator, such as HSPICE, is itself a MNA solver [60–63]. The drawback of the above-mentioned methods, therefore, is that they tried to reimplement what SPICE software already did inside an EM program, but probably is not as robust as SPICE software stands. All SPICE models, such as diodes and various types of transistors, have to be redefined in these EM-MNA solvers, as required for real industrial application purposes. Herein, we believe designing a hybrid EM-circuit algorithm with separated EM and circuit programs is a better way to address real-life applications. Because in this way, our EM program can connect with any available circuit program, so that we can utilize the circuit solvers, semiconductor models, and component definitions in existing software products or programs.

Lastly but perhaps the most importantly, we need to build the interface between the electromagnetic and circuit solvers. Existing work on DGTD and circuit co-simulation can be found in [51], where the authors formulated a lumped circuit subcell model to link DGTD with SPICE solver. The circuits were solved by calling external
SPICE software. Nevertheless, DGTD and SPICE were coupled through an explicit way and not connected rigorously. Therefore, the accuracy and performance of the method may become impaired in presence of highly nonlinear devices if a time step is not carefully chosen to be small enough.

In this work, we propose an EM-circuit co-simulation method by decompose an EM-circuit problem into two subsystems, one containing the EM structures, the other containing nonlinear circuits. The EM part is simulated in DGTD while the circuit part is simulated in a standalone SPICE or IBIS solver [61–69]. Planar surface ports are built to make the links between the two simulation programs. A self-consistent interfacing approach is developed to solve the problem in an iterative manner.

1.3 Organization

The rest of the dissertation is organized as follows.

Chapter 2 presents the core of the proposed embedded DDM. We start by giving the boundary value problem (BVP) statement of the underlying EM phenomena. For illustration, a typical problem is decomposed into a background and a subdomain of embedded meshes. The discretizations between the subdomains are completely nonconformal and they are solved by a standard single-domain FEM solver independently. To ensure the EM field solutions between the subdomains are continuous and consistent, we then establish the coupling sources between them. The background subdomain couples to the embedded meshes through field continuity sources on the subdomain interface. Meanwhile, the embedded subdomain imposes the coupling sources, which account for the material properties, PECs, and ports in it, onto the
background. Finally, the overall Galerkin statement and the corresponding discrete implementation are detailed.

In Chapter 3, we examine the numerical properties of the embedded DDM. Firstly, the scattering of a dielectric coated PEC sphere is presented, for the validation of the accuracy and iterative convergence. Moreover, the combination of embedded DDM and integral equation truncation is shown and compared to analytical reference. Secondly, we give a rectangular waveguide example with purposely designed interior PEC/port structures. The PEC/port structures are modeled as embedded subdomains while the background is the waveguide, so that we can verify our formulation of embedded PEC and port sources. Furthermore, mesh refinement study is conducted in this example in order to show the method’s h-convergence property. Thirdly, the implementation of the proposed approach is investigated through two numerical experiments, regarding the surface integration scheme on the subdomain interface and the TCs on the touched interfaces between embedded meshes. Special efforts are proposed to maintain the accuracy of the proposed method under certain circumstances.

Afterwards, Chapter 4 illustrates the applications of embedded DDM through three types of problems: the electromagnetic compatibility/interference of mobile devices near the human bodies, the simulation of complex antenna structures, and the signal integrity analyses of integrated circuits. We will show that, by adopting embedded DDM in repetitive simulations, spent efforts on discretizations and matrix assemblings/factorizations can be re-utilized, and complex EM analysis can be significantly eased. Moreover, the flexibility and robustness of embedded DDM will be clearly demonstrated.
In Chapter 5, we study time-domain computation and discusses the numerical simulation of mixed EM-circuit problems. A mixed system is divided into an EM subdomain and a circuit subdomain, then they are solved in separate programs. The EM subdomain is addressed by employing interior penalty DGTD formulation with the current input from the circuit engine. Meanwhile, the circuits are driven by the voltage source calculated from the EM side. By establishing circuit ports in the EM structure, we shall introduce a self-consistent looping scheme with detailed explanation of the coupling mechanism between the two simulators. To show the accuracy and reliability of the co-simulation approach, we present the computations of two real-life PCB models. One is a pulse generator, in which the DGTD-SPICE co-simulation are examined. The other is a seven-layer PCB system, where nonlinear IBIS models are integrated into the DGTD simulation.

Finally, the conclusions are made, and future directions of this research are discussed.
Chapter 2: Embedded Domain Decomposition Formulation

2.1 Boundary Value Problem (BVP) Statements

Electromagnetic phenomena are governed by Maxwell’s equations, subject to specific boundary conditions such as the Silver-Müller radiation condition. In deriving the algorithm of embedded DDM, we consider a bounded domain $\Omega \subset \mathbb{R}^3$, as shown in Figure 2.1. The first-order absorbing boundary condition (ABC) is imposed on $\partial \Omega$ to truncate the infinite domain into a finite one. Furthermore, there is a domain $\Omega_2$ inside domain $\Omega$ ($\Omega_2 \subset \Omega$). Herein, we assume the boundaries $\partial \Omega$ and $\partial \Omega_2$ are smooth so that both of them have well-defined unit outward normal at almost every point. The material properties $\epsilon_2(x), \mu_2(x)$ within $\Omega_2$ can be inhomogeneous and different from $\epsilon_1(x), \mu_1(x)$ within $\Omega \setminus \Omega_2$. Moreover, $\Omega_2$ may contain perfect electric conductors (PECs) and ports. The excitation of the problem can be an incident EM wave, an impressed electric current in $\Omega \setminus \Omega_2$, an impressed electric current in $\Omega_2$, or the combination of them.

Subsequently, assuming an $e^{j\omega t}$ dependence, we can write the time-harmonic BVP in Figure 2.1 as

$$\nabla \times \frac{1}{\mu_{r_1}} \nabla \times \mathbf{E} - k^2 \epsilon_{r_1} \mathbf{E} = -jk \eta \mathbf{J}_{1}^{\text{imp}} \quad \text{in } \Omega \setminus \Omega_2$$
Figure 2.1: A boundary value problem with the 1st order ABC.

\[
\nabla \times \frac{1}{\mu_{r_2}} \nabla \times \mathbf{E} - k^2 \varepsilon_{r_2} \mathbf{E} = -jk \eta \mathbf{J}_{\text{imp}}^{\text{imp}} \quad \text{in } \Omega_2
\]

\[
\pi_\tau^+(\frac{1}{\mu_{r_1}} \nabla \times \mathbf{E}) - \frac{jk}{\eta_{r_1}} \pi_\tau^+(\mathbf{E}) = \pi_\tau^+(\frac{1}{\mu_{r_1}} \nabla \times \mathbf{E}_{\text{inc}}) - \frac{jk}{\eta_{r_1}} \pi_\tau^+(\mathbf{E}_{\text{inc}}) \quad \text{on } \partial \Omega
\]

\[
\pi_\tau^+(\mathbf{E}) = 0 \quad \text{on } \Gamma_{\text{pec}}
\]

\[
\left[ \frac{1}{\mu_{r_1}} \nabla \times \mathbf{E} \right]_x = -jk \eta \mathbf{J}^{\text{port}} \quad \text{on } \Gamma_{\text{port}}
\]

where \( k = \omega \sqrt{\mu_0 \varepsilon_0} \) is the wave number of free space. The free-space intrinsic impedance is denoted as \( \eta = \sqrt{\mu_0 / \varepsilon_0} \). \( \varepsilon_{ri} \) and \( \mu_{ri} \) are, respectively, the relative permittivity and permeability of the medium, with \( \eta_{ri} = \sqrt{\mu_{ri} / \varepsilon_{ri}} \) defined as the relative wave impedance, and \( i \in \{1, 2\} \). The tangential components trace operator \( \pi_\tau(\cdot) \) and twisted tangential trace operator \( \pi_\times(\cdot) \) are adopted in our analysis, defined as

\[
\pi_\tau(\mathbf{u}) := \hat{n} \times \mathbf{u} \times \hat{n} \quad (2.2)
\]

\[
\pi_\times^+(\mathbf{u}) := \hat{n}^+ \times \mathbf{u} \quad (2.3)
\]

where \( \hat{n}^+ \) and \( \hat{n}^- \) are the unit outward normal and unit inward normal to \( \Omega \) or \( \Omega_2 \), respectively. \( \left[ \mathbf{u} \right]_x \) refers to the associated field jump across a surface like \( \Gamma_{\text{port}} \)

\[
\left[ \mathbf{u} \right]_x := \pi_\times^+(\mathbf{u}^+) + \pi_\times^-(\mathbf{u}^-) \quad (2.4)
\]
Refer to Figure 2.1, $\Gamma_p$ in $\Omega_2$ can be either $\Gamma_{\text{pec}}$ or $\Gamma_{\text{port}}$. $\Gamma_{\text{pec}}$ denotes the collection of PEC surfaces on which the tangential component of electric field vanishes. $\Gamma_{\text{port}}$ indicates the surface of internal port where a specific surface current density $J^\text{port}$ exists.

To facilitate later discussion, we shall define the function spaces for electromagnetic quantities. Let $L^2(\Omega)$ be the set of all square-integrable scalar functions in domain $\Omega \subset \mathbb{R}^3$. We can define the following familiar vector function spaces [22, 70]

\[
\mathbf{H}(\text{curl}; \Omega) := \left\{ \mathbf{u} \in \left( L^2(\Omega) \right)^3 \mid \nabla \times \mathbf{u} \in \left( L^2(\Omega) \right)^3 \right\}
\]

\[
\mathbf{H}(\text{div}; \Omega) := \left\{ \mathbf{u} \in \left( L^2(\Omega) \right)^3 \mid \nabla \cdot \mathbf{u} \in L^2(\Omega) \right\}
\]

\[
\mathbf{H}^{-1/2}(\text{curl}; \partial \Omega) := \{ \pi_\tau(\mathbf{u}) \mid \mathbf{u} \in \mathbf{H}(\text{curl}; \Omega) \}
\]

\[
\mathbf{H}^{-1/2}(\text{div}; \partial \Omega) := \{ \pi_\times(\mathbf{u}) \mid \mathbf{u} \in \mathbf{H}(\text{curl}; \Omega) \}
\]

where $\mathbf{H}(\text{curl}; \Omega)$ corresponds to the space of finite-energy solutions in which the electric field $\mathbf{E}$ resides. In order to simplify notation, we further introduce the volume and surface inner products as

\[
(\mathbf{u}, \mathbf{v})_\Omega := \int_{\Omega} \mathbf{u} \cdot \mathbf{v} dV \tag{2.5}
\]

for $\mathbf{u}, \mathbf{v} \in (L^2(\Omega))^3$, and

\[
(\mathbf{u}, \mathbf{v})_{\partial \Omega} := \int_{\partial \Omega} \mathbf{u} \cdot \mathbf{v} dA \tag{2.6}
\]

for $\mathbf{u}, \mathbf{v} \in (L^2(\partial \Omega))^3$.

### 2.2 Embedded Domain Decomposition

As mentioned earlier, our goal is to decompose the problem into several simpler subproblems with shared regions, treat the subproblems separately, and provide an
interface method to couple them. To explain our basic strategy, we consider a simple setting by decomposing the original domain $\Omega$ into a background subdomain $\Omega_1$ and an embedded subdomain $\Omega_2$. The two subdomains have a common region, as shown in Figure 2.2.

![Figure 2.2: Embedded domain decomposition scheme for an electromagnetic problem.](image)

Note the shape of $\Omega_1$ is the same as $\Omega$ except the region inside $\partial \Omega_2$, which now contains no geometrical information of $\Omega_2$ and is set to be filled with the same material as in $\Omega \setminus \Omega_2$. The initial decomposed BVP statements of the subdomains, without consideration of the coupling between them, can be written as

$$
\nabla \times \frac{1}{\mu_r} \nabla \times E_1 - k^2 \epsilon_r E_1 = -j k \eta J_1^{\text{imp}} \quad \text{in } \Omega_1
$$

$$
\pi^+_x \left( \frac{1}{\mu_r} \nabla \times E_1 \right) - \frac{j k}{\eta_r} \pi_\tau (E_1) = \pi^+ \left( \frac{1}{\mu_r} \nabla \times E_1^{\text{inc}} \right) - \frac{j k}{\eta_r} \pi_\tau (E_1^{\text{inc}}) \quad \text{on } \partial \Omega_1 \quad (2.7)
$$

for the background subdomain $\Omega_1$, and

$$
\nabla \times \frac{1}{\mu_r} \nabla \times E_2 - k^2 \epsilon_r E_2 = -j k \eta J_2^{\text{imp}} \quad \text{in } \Omega_2
$$
\[
\pi_r(\mathbf{E}_2) = 0 \quad \text{on } \Gamma_{\text{pec}}
\]
\[
\left[ \frac{1}{\mu_r} \nabla \times \mathbf{E}_2 \right] \times = -j k \eta J_{\text{port}}^{\text{port}} \quad \text{on } \Gamma_{\text{port}} \quad (2.8)
\]

for the embedded subdomain \( \Omega_2 \), where \( \mathbf{E}_i \) represents the electric field in subdomain \( \Omega_i \), \( i \in \{1, 2\} \).

Then, we construct appropriate meshes for each of them. It is worth mentioning that the meshing processes of \( \Omega_1 \) and \( \Omega_2 \) are completely independent. In other words, \( \Omega_1 \) has no prior information about the geometries, material properties, PECs and ports in \( \Omega_2 \), nor does \( \Omega_2 \) have prior information about \( \Omega_1 \). Consequently, the discretization of \( \Omega_2 \) can be significantly different from that of \( \Omega_1 \) at the same spatial position. At this point, it should become evident that the manner of information communication between the subdomains is the crucial step of the proposed method. In the following, we will discuss two directions of information flow. One is to transfer field information from \( \Omega_1 \) to \( \Omega_2 \). The other is to send to \( \Omega_1 \) the information of material properties, PECs, and ports in \( \Omega_2 \).

### 2.3 Field Coupling From \( \Omega_1 \) to \( \Omega_2 \)

In order to transfer the field information from the background subdomain \( \Omega_1 \) to the embedded subdomain \( \Omega_2 \), and obtain a self-consistent solution inside \( \partial \Omega_2 \), the field continuity at the boundary \( \partial \Omega_2 \) between \( \Omega_1 \) and \( \Omega_2 \) should be observed.

First, we denote the subdomain interface as \( \Gamma_{12} (= \partial \Omega_2) \) and define a vector auxiliary variable to represent the scaled surface electric current on it

\[
\mathbf{j}_2 := \frac{1}{k} \pi_r^+ \left( \frac{1}{\mu_r} \nabla \times \mathbf{E}_2 \right) \quad (2.9)
\]
Figure 2.3: Field continuity enforcement across the subdomain interface.

In order to perform field communication across $\Gamma_{12}$, we can employ the Robin-type transmission condition as

$$kj_2 - jk\frac{1}{\bar{\eta}_r} \pi_\tau(E_2) = \pi_\times^+ \left( \frac{1}{\mu_{r1}} \nabla \times E_1 \right) - jk\frac{1}{\bar{\eta}_r} \pi_\tau(E_1) \quad \text{on} \quad \Gamma_{12} \quad (2.10)$$

where $\bar{\eta}_r = \sqrt{(\mu_{r1} + \mu_{r2})/(\epsilon_{r1} + \epsilon_{r2})}$. The proper space for $j_2$ should be $H^{-1/2}(\text{div}_\tau; \Gamma_{12})$, the space of normally continuous surface vector functions. Denoting $v_2 \in H(\text{curl}; \Omega_2)$ as the electric field in $\Omega_2$, we can test the above transmission condition with the vector field $\pi_\tau(v_2) \in H^{-1/2}(\text{curl}_\tau; \Gamma_{12})$ and obtain the following

$$\left\langle \pi_\tau(v_2), k j_2^{(n)} - jk\frac{1}{\bar{\eta}_r} \pi_\tau(E_2^{(n)}) \right\rangle_{\Gamma_{12}} =$$

$$\left\langle \pi_\tau(v_2), \pi_\times^+ \left( \frac{1}{\mu_{r1}} \nabla \times E_1^{(n)} \right) - jk\frac{1}{\bar{\eta}_r} \pi_\tau(E_1^{(n)}) \right\rangle_{\Gamma_{12}} \quad (2.11)$$

where the superscript $(n)$ means the $n$-th iteration in DDM.
However, the direct evaluation of the integral term at the right hand side of (2.11) is hardly feasible because $\pi_\tau(v_2)$ and $\left[\pi_\times^+\left(\mu_{r_1}^{-1}\nabla \times E_1^{(n)}\right) - jk\eta_{r_1}^{-1}\pi_\tau\left(E_1^{(n)}\right)\right]$ are not defined on the same discretization. Our approach will be based on the use of triangulation available from the mesh of $\Omega_2$. Let $h$ denotes the characteristic element size in the finite element mesh $\Omega_1^h$ and the surface triangulation $\Gamma_{12}^h$, with $E_1^h$ and $v_2^h$ being the discrete trial and test functions. Moreover, let $w_1$ and $w_2$ be the interpolatory curl-conforming basis functions inside $\Omega_1^h$ and $\Omega_2^h$, respectively, such that $E_1^h = \sum_i e_{1,i}w_{1,i}$ in the tetrahedrons of $\Omega_1^h$ and $\pi_\tau(v_2^h) = \sum_i e_{2,i}\pi_\tau(w_{2,i})$ in the triangles of $\Gamma_{12}^h$, where $e_1, e_2$ are the coefficients of basis functions. Subsequently, the integral can be approximated by using Gaussian quadrature on the triangular mesh of $\Gamma_{12}^h$, as follows

$$\left\langle \pi_\tau(v_2^h), \pi_\times^+\left(\mu_{r_1}^{-1}\nabla \times E_1^{h,(n)}\right) - jk\eta_{r_1}^{-1}\pi_\tau\left(E_1^{h,(n)}\right)\right\rangle_{\Gamma_{12}^h} = \sum_j e_2 \sum_i \tilde{w}_{2,i} \cdot \left[\pi_\times^+\left(\mu_{r_1}^{-1}\nabla \times w_{1,i}\right)\right] w_i e_1^{(n)} \Delta_j$$

(2.12)

where $j$ is the index of the triangles on $\Gamma_{12}^h$, $\Delta_j$ is the area of the $j$-th triangle, $i$ is the index of Gaussian quadrature points in each triangle, and $w_i$ is the weight associated with $i$-th Gaussian point. Moreover, $\tilde{\cdot}$ denotes a column vector and $\cdot$ denotes a row vector.

The computation of (2.12) requires to find out in which tetrahedron of $\Omega_1^h$ each Gaussian quadrature point of $\Gamma_{12}^h$ is located. To search a point location with respect to a group of tetrahedron is an operation of complexity $O(\log N)$, where $N$ is the number of tetrahedrons in $\Omega_1^h$. If $\Gamma_{12}^h$ consists of $M$ triangles and the number of Gaussian quadrature points is $p$, the overall complexity of location detection is $O(pM \log N)$. More specifically, for $\Omega_1^h$ an octree of nested boxes can be created, wherein each box is
Figure 2.4: Post-processing step to sample the field solutions in the tetrahedrons of $\Omega_1$.

subdivided into, and linked to, smaller child boxes. Each box of the tree leaf contains the tetrahedrons of $\Omega_1^h$. To find the location of a Gaussian quadrature point in $\Omega_1^h$ is to traverse the octree. Besides, the process is highly parallelizable because the search of each point is independent. Therefore, the spatial relationship between the Gaussian quadrature points and the tetrahedrons can be fast established.

In terms of implementation, once the local FEM simulation of $\Omega_1$ is finished at the $n$-th iteration, we perform a post-processing step to sample the electric and magnetic fields of $\Omega_1$. The sampling points are the Gaussian quadrature points in the triangles of $\Gamma_{12}$. In this way, the integral (2.12) can be evaluated and used for the local FEM simulation of $\Omega_2$ at the $n$-th iteration.

2.4 Coupling From $\Omega_2$ to $\Omega_1$

2.4.1 Coupling Sources of Material Difference

As stated in previous sections, we assume the material properties of the embedded subdomain $\Omega_2$ is different from those of the background domain $\Omega_1$ inside $\partial\Omega_2$. Our
Figure 2.5: Modified volume sources representing the material difference between $\Omega_1$ and $\Omega_2$.

goal here is to perform necessary modification to the BVP (2.7) in $\Omega_1$ so as to account for the information of material properties from $\Omega_2$ to $\Omega_1$.

Assuming that $\mathbf{E}_2$ and $\mathbf{H}_2$ are the electric field and magnetic field solutions which satisfy the BVP of $\Omega_2$, we insert two modified terms $j\omega (\epsilon_2 - \epsilon_1) \mathbf{E}_2$ and $j\omega (\mu_2 - \mu_1) \mathbf{H}_2$ into the original Maxwell’s equations in $\Omega_1$ as

\begin{align}
\nabla \times \mathbf{E}_1 &= -j\omega \mu_1 \mathbf{H}_1 - j\omega (\mu_2 - \mu_1) \mathbf{H}_2 \quad (2.13) \\
\nabla \times \mathbf{H}_1 &= j\omega \epsilon_1 \mathbf{E}_1 + j\omega (\epsilon_2 - \epsilon_1) \mathbf{E}_2 + \mathbf{J}_1^{\text{imp}} \quad (2.14)
\end{align}

In the above equations, $j\omega (\epsilon_2 - \epsilon_1) \mathbf{E}_2$ and $j\omega (\mu_2 - \mu_1) \mathbf{H}_2$ can be viewed as the electric and magnetic polarizations caused by the change of material properties from $\epsilon_{r1}$, $\mu_{r1}$ to $\epsilon_{r2}$, $\mu_{r2}$. Subsequently, equations (2.13) and (2.14) constitute a modified
vector wave equation for the electric field in $\Omega_1$, as follows

$$\nabla \times \frac{1}{\mu_r} \nabla \times E_1 - k^2 \epsilon_r E_1 = -jk\eta J_{1}^{\text{imp}} + G_{12} + F_{12} \quad (2.15)$$

Herein, we introduce two modified sources $F$ and $G$ as

$$F_{12} = -k^2 (\epsilon_r - \epsilon_r) E_2 \quad (2.16)$$

$$G_{12} = \nabla \times \left( \frac{1}{\mu_r} - \frac{1}{\mu_r} \right) \nabla \times E_2 \quad (2.17)$$

In this way, the solution of the electric field in $\Omega_1$ is affected by the volume sources $F_{12}$ and $G_{12}$, which account for the material difference between $\Omega_1$ and $\Omega_2$.

We proceed to test the modified vector wave equation with the electrical field $v_1 \in H(\text{curl}; \Omega_1)$. Through the application of divergence theorem and integration by part, we have

$$\left( \nabla \times v_1, \frac{1}{\mu_r} \nabla \times E_1^{(n)} \right)_{\Omega_1} - k^2 \left( v_1, \epsilon_r E_1^{(n)} \right)_{\Omega_1} + k \left( \pi_r (v_1), J_{1}^{(n)} \right)_{\partial \Omega_1} =$$

$$-jk\eta \left( v_1, J_{1}^{\text{imp}} \right)_{\Omega_1} + \left( v_1, G_{12}^{(n-1)} \right)_{\Omega_2} + \left( v_1, F_{12}^{(n-1)} \right)_{\Omega_2} \quad (2.18)$$
in which $J_1^{(n)} \in H^{-1/2}(\text{div}; \partial \Omega_1)$. Similar to (2.11), $(v_1, G_{12}^{(n-1)})_{\Omega_2}$ and $(v_1, F_{12}^{(n-1)})_{\Omega_2}$ require inner products of quantities defined on different discretizations. Therefore, we perform the integration by employing the tetrahedron meshes available in $\Omega_2$ and adopting the Gaussian quadrature integration in tetrahedron, as shown in Figure 2.6.

Consequently, with the simulation results of $\Omega_2$ at the $(n-1)$-th iteration, we can construct the modified sources $F_{12}$ and $G_{12}$ at the Gaussian quadrature points in the tetrahedrons of $\Omega_2$, so long as material difference exists. These sources are imposed onto $\Omega_1$ and will be used for the local FEM simulation in $\Omega_1$ at the $n$-th iteration.

### 2.4.2 Coupling Sources of PEC and Port

In addition to material properties, we also need to properly transfer the PEC and port conditions from $\Omega_2$ to $\Omega_1$. Conventionally, FEM defines the Dirichlet boundary condition $\pi_{\tau}(E_1) = 0$ on the triangulation of the PEC surfaces, which also implies a magnetic field discontinuity between adjacent tetrahedrons. However, we face a challenge here that the triangular mesh of $\Omega_1$ may not be conformal to the geometry of the PEC surface of $\Omega_2$, since the discretizations of the subdomains are totally independent. Due to the interpolatory property of curl-conforming basis function that we use in the tetrahedral element of $\Omega_1$, it is not easy to straightforwardly implement $\pi_{\tau}(E_1) = 0$ inside a tetrahedron in $\Omega_1$, because the magnetic field discontinuity cannot be ensured.

To overcome this difficulty, we employ an alternative approach, in which the tangential electric field on PEC is not explicitly constrained to be zero. Because of the surface equivalent theorem, a PEC object can be transformed into an equivalent problem where $J_{\text{pec}}$ and zero magnetic current reside on the boundary surface of
the PEC. For this reason, we shall model the PECs of the embedded subdomains as current surfaces in the background subdomain. The other essential ingredient in the embedded region, port, can be characterized by the surface current density on it and is associated with the magnetic field jump across the port surface. Therefore, we also utilize current surface for the implementation of port condition. The corresponding Galerkin statement for PEC and port is

\[
\left( \nabla \times \mathbf{v}_1, \frac{1}{\mu_\tau 1} \nabla \times \mathbf{E}_{1}^{(n)} \right)_{\Omega_1} - k^2 \left( \mathbf{v}_1, \epsilon_\tau 1 \mathbf{E}_{1}^{(n)} \right)_{\Omega_1} + k \left\langle \pi_\tau (\mathbf{v}_1), \mathbf{j}_1^{(n)} \right\rangle_{\partial \Omega_1} \\
= -jk \eta \left\langle \pi_\tau (\mathbf{v}_1), \mathbf{j}_{\text{pec}}^{(n-1)} \right\rangle_{\Gamma_{\text{pec}}} - jk \eta \left\langle \pi_\tau (\mathbf{v}_1), \mathbf{j}_{\text{port}}^{(n-1)} \right\rangle_{\Gamma_{\text{port}}}
\]

(2.19)

where \( \mathbf{v}_1 \in \mathbf{H}(\text{curl}; \Omega_1) \), \( \mathbf{j}_1^{(n)} \in \mathbf{H}^{-1/2}(\text{div}; \partial \Omega_1) \), and \( \mathbf{j}_{\text{pec}}^{(n-1)}/\mathbf{j}_{\text{port}}^{(n-1)} \) represents the current on the PEC/port surface of \( \Omega_2 \) at the \((n - 1)\)-th iteration.

As can be inspected in (2.19), \( \left\langle \pi_\tau (\mathbf{v}_1), \mathbf{j}_{\text{pec}}^{(n-1)} \right\rangle \) and \( \left\langle \pi_\tau (\mathbf{v}_1), \mathbf{j}_{\text{port}}^{(n-1)} \right\rangle \) indicate the reactions of the field \( \mathbf{E}_1 \) on the sources \( \mathbf{j}_{\text{pec}}^{(n-1)} \) and \( \mathbf{j}_{\text{port}}^{(n-1)} \). To compute them appropriately, we choose a closed surface in \( \Omega_2 \) that fully encloses all the PECs and ports. The surface is chosen based on the available triangular mesh in \( \Omega_2 \) and we denote it by \( \Gamma_{21} \). Moreover, the tetrahedral region inside \( \Gamma_{21} \) are represented as \( \Omega'_2 (\Omega'_2 \subseteq \Omega_2) \).
Subsequently, the BVP for the region $\Omega'_2$ can be listed as

$$\nabla \times \left( \frac{1}{\mu_r} \nabla \times \mathbf{E}_2 \right) - k^2 \varepsilon_r \mathbf{E}_2 = 0 \quad \text{in } \Omega'_2,$$

$$[\mathbf{H}_2]_\times = \mathbf{J}_{\text{pec}} \quad \text{on } \Gamma_{\text{pec}}$$

$$[\mathbf{H}_2]_\times = \mathbf{J}_{\text{port}} \quad \text{on } \Gamma_{\text{port}} \quad (2.20)$$

Through the applications of reaction pairing [71] and the interior penalty approach [72], we can derive the Galerkin statement for $\Omega'_2$ at the $(n-1)$-th iteration as

$$\left( \nabla \times \mathbf{v}_1, \frac{1}{\mu_r} \nabla \times \mathbf{E}_2^{(n-1)} \right)_{\Omega'_2} - k^2 \left( \mathbf{v}_1, \varepsilon_r \mathbf{E}_2^{(n-1)} \right)_{\Omega'_2}$$

$$+ c_1 \left( \pi_{\tau}(\mathbf{v}_1), \left[ \mathbf{H}_2 \right]_\times^{(n-1)} - \mathbf{J}_{\text{pec}}^{(n-1)} \right)_{\Gamma_{\text{pec}}}$$

$$+ c_2 \left( \pi_{\tau}(\mathbf{v}_1), \left[ \mathbf{H}_2 \right]_\times^{(n-1)} - \mathbf{J}_{\text{port}}^{(n-1)} \right)_{\Gamma_{\text{port}}} = 0 \quad (2.21)$$

where the electrical field in $\Omega_1$ is adopted as the test function. With $c_1 = c_2 = -jk\eta$, we can further obtain

$$\left( \pi_{\tau}(\mathbf{v}_1), \mathbf{J}_{\text{pec}}^{(n-1)} \right)_{\Gamma_{\text{pec}}} + \left( \pi_{\tau}(\mathbf{v}_1), \mathbf{J}_{\text{port}}^{(n-1)} \right)_{\Gamma_{\text{port}}} =$$
\[
\left( \nabla \times v_1, H_2^{(n-1)} \right)_{\Omega_2'} - j\omega \left( v_1, \epsilon_2 E_2^{(n-1)} \right)_{\Omega_2'} + \left\langle \pi_\tau(v_1), \pi_\chi^+(H_2^{(n-1)}) \right\rangle_{\Gamma_{21}}
\]  
(2.22)

In such a manner, the PECs and ports of \( \Omega_2 \) are embedded into the background subdomain \( \Omega_1 \) by coupling the reaction integrals from (2.22) to (2.19).

To calculate (2.22), we utilize tetrahedral Gaussian quadrature integration for the evaluation of \( \left( \nabla \times v_1, H_2^{(n-1)} \right) \) and \( \left( v_1, \epsilon_2 E_2^{(n-1)} \right) \), while \( \left\langle \pi_\tau(v_1), \pi_\chi^+(H_2^{(n-1)}) \right\rangle \) will be integrated numerically based on the triangular meshes on \( \Gamma_{21} \).

Note that in the above formulation, we follow the principle to form reaction pairings [12] such that the integrals like \( \left\langle \pi_\tau(v_1), J_{\text{pec}}^{(n-1)} \right\rangle_{\Gamma_{\text{pec}}} \) and \( \left\langle \pi_\tau(v_1), J_{\text{port}}^{(n-1)} \right\rangle_{\Gamma_{\text{port}}} \) have the appropriate physical meaning of \( \mathbf{E} \cdot \mathbf{J} \). Hence, they are related to the power generated by the surface current \( J_{\text{pec}}^{(n-1)} \) on PEC or \( J_{\text{port}}^{(n-1)} \) on port. As the surface current is embedded in \( \Omega_1 \), the power generated by \( J_{\text{pec}}^{(n-1)} \) and \( J_{\text{port}}^{(n-1)} \) from \( \Omega_2 \) radiates into \( \Omega_1 \). From such a perspective, we are actually performing the power coupling from subdomain \( \Omega_2 \) to subdomain \( \Omega_1 \).

### 2.5 Discrete Formulation

Let \( \Omega_i^h (i \in \{1, 2\}) \) denote the independent tetrahedral mesh of each subdomain \( \Omega_i \), where \( h \) is the characteristic edge length. \( \Gamma_i^h, \Gamma_{12}^h, \) and \( \Gamma_{21}^h \) are the surface triangulations induced on \( \Gamma_1, \Gamma_{12}, \) and \( \Gamma_{21} \), respectively. Moreover, the corresponding volume mesh in \( \Omega_2' \) is represented by \( \Omega_2'^{h} \).

In each subdomain, we define the discrete trial and test functions as \( \mathbf{E}_i^h \in \mathbf{X}_i^h \) and \( v_i^h \in \mathbf{X}_i^h \), respectively, with \( \mathbf{X}_i^h \subset \mathbf{H}(\text{curl}; \Omega_i) \). Here, \( \mathbf{X}_i^h \) is taken to be the space spanned by the mixed-order curl-conforming vector basis functions over \( \Omega_i^h \) [20, 73], with order \( p = 2 \). On the surface \( \partial \Omega_i^h \), we further employ the discrete vector trial functions as \( \mathbf{j}_i^h \in \mathbf{Y}_i^h \), with \( \mathbf{Y}_i^h \subset \mathbf{H}^{-1/2}(\text{div}; \partial \Omega_i) \). \( \mathbf{Y}_i^h \) corresponds to the
two-dimensional restriction of $X^h_1$, but the degrees of freedom (DOFs) are assigned independently for the surface.

Subsequently, the discrete Galerkin formulation for the proposed embedded DDM can be formally stated as:

Find $(E_1^{h,(n)}, E_2^{h,(n)}) \in X^h_1 \times X^h_2$ and $(J_1^{h,(n)}, J_2^{h,(n)}) \in Y^h_1 \times Y^h_2$, such that

\[
\begin{align*}
    &a_1(v_1^h, E_1^{h,(n)}) + a_2(v_2^h, E_2^{h,(n)}) - \mathcal{J}_1(v_1^h) - \mathcal{J}_2(v_2^h) \\
    &+ k \left\langle \pi_\tau(v_1^h), J_1^{h,(n)} \right\rangle_{\partial \Omega^h_i} + k \left\langle \pi_\tau(v_2^h), J_2^{h,(n)} \right\rangle_{\partial \Omega^h_i} \\
    &+ \left\langle \pi_\tau(v_1^h), k J_1^{h,(n)} \right\rangle_{\Gamma_{12}^h} - jk \frac{1}{\eta_1} \pi_\tau(E_1^{h,(n)}) \bigg|_{\partial \Omega^h_i} \\
    &- \left\langle \pi_\tau(v_1^h), \pi_\times \left( \frac{1}{\mu_1} \nabla \times E_1^{inc} \right) \right\rangle_{\Gamma_{12}^h} - jk \frac{1}{\eta_1} \pi_\tau(E_1^{inc}) \\
    &+ \left\langle \pi_\tau(v_2^h), J_2^{h,(n)} \right\rangle_{\Gamma_{12}^h} - jk \frac{1}{\eta_1} \pi_\tau(E_2^{h,(n)}) \\
    &- \left( v_1^h, G_{12}^{(n-1)} \right)_{\Omega^h_2} - \left( v_1^h, F_{12}^{(n-1)} \right)_{\Omega^h_2} \\
    &+ jk \eta \left\langle \pi_\tau(v_1^h), J^{(n)}_{\text{pec}/\Gamma_{\text{pec}}} \right\rangle_{\Gamma_{\text{pec}}} + jk \eta \left\langle \pi_\tau(v_1^h), J^{(n)}_{\text{port}/\Gamma_{\text{port}}} \right\rangle_{\Gamma_{\text{port}}} = 0
\end{align*}
\]

\[
\forall (v_1^h, v_2^h) \in X^h_1 \times X^h_2.
\]

with

\[
\begin{align*}
    a_i(v, u) &= \left( \nabla \times v, \frac{1}{\mu_{ri}} \nabla \times u \right)_{\Omega^h_i} - k^2 (v, \epsilon_{ri} u)_{\Omega^h_i} \\
    \mathcal{J}_i(v) &= -jk \eta \left( v, J^{\text{imp}}_i \right)_{\Omega^h_i} \\
    F_{12}^{(n)} &= -k^2 (\epsilon_{r1} - \epsilon_{r2}) E_2^{h,(n)} \\
    G_{12}^{(n)} &= \nabla \times \left( \frac{1}{\mu_1} - \frac{1}{\mu_2} \right) \nabla \times E_2^{h,(n)} \\
    \left\langle \pi_\tau(v_1^h), J^{(n)}_{\text{pec}/\Gamma_{\text{pec}}} \right\rangle_{\Gamma_{\text{pec}}} + \left\langle \pi_\tau(v_1^h), J^{(n)}_{\text{port}/\Gamma_{\text{port}}} \right\rangle_{\Gamma_{\text{port}}} \\
    &= \left( \nabla \times v_1^h, H_2^{h,(n)} \right)_{\Omega^h_2} - j\omega \left( v_1^h, \epsilon_{2} E_2^{h,(n)} \right)_{\Omega^h_2}
\end{align*}
\]
Next, we expand the vector fields by the corresponding basis functions. The discrete system then can be expressed as a matrix equation

\[
\begin{pmatrix}
    A_1 & -C_{12} \\
    -C_{21} & A_2
\end{pmatrix}
\begin{pmatrix}
    x_1^{(n)} \\
    x_2^{(n)}
\end{pmatrix} =
\begin{pmatrix}
    b_1^{(n)} \\
    b_2^{(n)}
\end{pmatrix}
\]

with

\[
A_i = \begin{pmatrix}
    A_{iH} & A_{iB} \\
    A_{iB} & A_{iB} \\
    0 & T_{ii}^{ee} + T_{ii}^{ej}
\end{pmatrix}, \quad x_1 = \begin{pmatrix}
    e_1 \\
    j_1
\end{pmatrix}, \quad e_i = \begin{pmatrix}
    e_{1i} \\
    e_{B1}
\end{pmatrix}, \quad j_i = \begin{pmatrix}
    j_{1i} \\
    j_{B1}
\end{pmatrix}
\]

\[
x_2 = \begin{pmatrix}
    e_{21} \\
    e_{2B}
\end{pmatrix}, \quad C_{21} = \begin{pmatrix}
    0 & 0 \\
    0 & 0 \\
    0 & T_{21}^{ee} + T_{21}^{ej}
\end{pmatrix}
\]

\[
b_1 = \begin{pmatrix}
    y_1 \\
    y_{1inc}
\end{pmatrix}, \quad b_2 = \begin{pmatrix}
    y_2 \\
    0
\end{pmatrix}
\]

where \( e_i \) is the solution vector which collects the coefficients of curl-conforming basis functions over \( \Omega_i^h \), and \( j_i \) is the coefficient vector associated with surface div-conforming basis functions on \( \partial\Omega_i^h \). The superscript \( x \in \{I, B\} \) corresponds, respectively, to entities that are completely inside \( \Omega_i^h \) and those residing on the boundary \( \partial\Omega_i^h \). Furthermore, we use the superscript \( M \) to represent the unknowns/matrices associated with the coupling source \( F_{12} \) and \( G_{12} \), and the superscript \( P \) to indicate the unknowns/matrices involved in the calculation of \( \langle \pi_\tau(v_1), J_{pec} \rangle \) and \( \langle \pi_\tau(v_1), J_{port} \rangle \). Moreover, \(^{(n)}\) represents the solution at the \( n \)-th iteration in the iterative process.
The block matrices are given by

\[
\begin{align*}
\tilde{x}_i^{(n)} A_{i} x_{i}^{(n)} &= a_i \left( E_i^h, E_i^{h,(n)} \right) \\
\tilde{x}_i^{(n)} T_{11}^{-1} \tilde{x}_{i}^{(n)} &= -j k \left\langle \pi_\tau \left( E_i^h \right), \frac{1}{\eta_r} \pi_\tau \left( E_i^{h,(n)} \right) \right\rangle_{\partial \Omega_i^h} \\
\tilde{x}_2^{(n)} T_{22}^{-1} \tilde{x}_{2}^{(n)} &= -j k \left\langle \pi_\tau \left( E_2^h \right), \frac{1}{\eta_r} \pi_\tau \left( E_2^{h,(n)} \right) \right\rangle_{\partial \Omega_2^h} \\
\tilde{x}_i^{(n)} T_{ij} \tilde{x}_j^{(n)} &= k \left\langle \pi_\tau \left( E_i^h \right), J_i^{h,(n)} \right\rangle_{\partial \Omega_i^h} \\
\tilde{x}_2^{(n)} T_{21} \tilde{x}_1^{(n)} &= -j k \left\langle \pi_\tau \left( E_2^h \right), \frac{1}{\eta_r} \pi_\tau \left( E_1^{h,(n)} \right) \right\rangle_{\partial \Omega_2^h} \\
\tilde{x}_2^{(n)} T_{12} \tilde{x}_2^{(n)} &= \left\langle \pi_\tau \left( E_2^h \right), \pi_\times \left( \frac{1}{\mu_r} \nabla \times E_1^{n-1} \right) \right\rangle_{\partial \Omega_2^h} + \left( E_1^h, F_1^{(n-1)} \right)_{\Omega_2^h} \\
\tilde{x}_i^{(n)} T_{12} \tilde{x}_2^{(n)} &= -j k \eta \left\langle \pi_\tau \left( E_1^h \right), J_{\text{pec}}^{(n)} \right\rangle_{\Gamma_{\text{pec}}} - j k \eta \left\langle \pi_\tau \left( E_1^h \right), J_{\text{port}}^{(n)} \right\rangle_{\Gamma_{\text{port}}} \\
\tilde{x}_i^{(n)} y_{i} &= J_i \left( E_i^h \right) \\
\tilde{x}_i^{(n)} y_{\text{inc}} &= \left\langle \pi_\tau \left( E_1^h \right), \pi_\times \left( \frac{1}{\mu_r} \nabla \times E_1^{\text{inc}} \right) \right\rangle_{\partial \Omega_i^h} \\
&\quad - j k \left\langle \pi_\tau \left( E_1^h \right), \frac{1}{\eta_r} \pi_\tau \left( E_1^{\text{inc}} \right) \right\rangle_{\partial \Omega_i^h} 
\end{align*}
\]  

In the global system matrix, the block matrices $A_1$ and $A_2$ in the diagonal stand for the FEM matrices of subdomain $\Omega_1$ and $\Omega_2$, respectively. The off-diagonal matrices $C_{12}$ and $C_{21}$ act as the couplings between the subdomains, determined by the Robin TC, polarization currents, surface current on PEC/port, and spatial relation between the subdomains.

To solve the discrete system (2.25), we use a preconditioned Krylov subspace method [12]. The symmetric block Gaussian-Seidel matrix is adopted as the preconditioner, with which the preconditioned system can be written as

\[
P^{-1} A x^{(n)} = P^{-1} b^{(n)} \]
The application of the preconditioner requires the inversion of the subdomain matrices $A_1$ and $A_2$. In this work, we perform the factorization of the subdomain matrices by using the multifrontal solution process [74]. The solution of the resulting partial differential equations (PDEs) is then obtained by employing the generalized conjugate residual (GCR) method [75,76].

Note that although we restrict our discussion to the case of two subdomains, the theory described above can be generalized to the computation of more than two subdomains as well, as depicted in Figure 2.9. If the embedded subdomains do not touch each other, such as $\Omega_2$ and $\Omega_4$, the formulation is already applicable because the coupling sources can be constructed separately for each subdomain. If the embedded subdomains have touching interfaces and are required to be touched physically in practical designs, such as $\Omega_2$ and $\Omega_3$, we can group the touched subdomains together as a big embedded subdomain, as displayed in Figure 2.10. Nonoverlapping TCs will

$$P = \begin{pmatrix} A_1 & 0 \\ -C_{21} & A_2 \end{pmatrix} \begin{pmatrix} A_1^{-1} & 0 \\ 0 & A_2^{-1} \end{pmatrix} \begin{pmatrix} A_1 & -C_{12} \\ 0 & A_2 \end{pmatrix}$$

(2.28)
be applied for the touching interfaces $\Gamma_{23}$ and $\Gamma_{32}$. Subsequently, the couplings between the background and big embedded subdomains can be established similarly to one embedded subdomain. The necessity to construct the coupling on the touching interface will be explained in Chapter 3. As for the corresponding discrete implementation, $A_2$ in (2.25) will be replaced by the system matrix of nonoverlapping DDM. The interested reader is referred to [15,16] for a detailed description.

In addition, we use the first order ABC for simplicity in the derivation. Nevertheless, the proposed method can be straightforwardly integrated with perfectly matched layer (PML) or boundary integral equation based truncations.
Chapter 3: Numerical Studies of Embedded Domain Decomposition

With the formulation in Chapter 2, we shall study the numerical properties of embedded DDM in this chapter, including the accuracy, iterative convergence, and h-convergence. Furthermore, the numerical implementations are investigated through two experiments. One is about the surface integration scheme on $\Gamma_{21}$. The other examines the couplings between touched embedded subdomains.

In all the following examples, we apply embedded DDM and solve the resulting system with the preconditioned GCR solver. Moreover, a relative residual is defined as

$$\epsilon^{(n)} = \frac{\|P^{-1}b^{(n)} - P^{-1}Ax^{(n)}\|_2}{\|P^{-1}b^{(n)}\|_2}$$

and is used as the convergence criteria for the GCR solver. $\epsilon = 10^{-3}$ is used in the examples unless otherwise specified. As comparison, we include reference results in order to validate the accuracy of embedded DDM. The reference results are obtained by solving the same problems with a standard single-domain FEM solver.

3.1 Scattering of a Dielectric-Coated PEC Sphere

In this example, we study the iterative convergence and accuracy of the proposed method. A plane wave is incident upon a dielectric-coated PEC sphere. The diameter
Figure 3.1: Embedded DDM settings for the scattering of a dielectric-coated PEC sphere: (a) subdomain $\Omega_1$; (b) subdomain $\Omega_2$ with an air buffer; (c) subdomain $\Omega_2$ without an air buffer.

of the PEC sphere is $2/3\lambda_0$ while the coating thickness is $1/6\lambda_0$, where $\lambda_0$ is the free-space wavelength. The relative permittivity of the coating is $\epsilon_r = 3$.

In applying embedded DDM to solve this problem, we use two subdomains $\Omega_1$ and $\Omega_2$ for discretization. $\Omega_1$ is chosen as a $5/3\lambda_0 \times 5/3\lambda_0 \times 5/3\lambda_0$ air box, and the first-order ABC is adopted on $\partial\Omega_1$. $\Omega_2$ contains the PEC sphere and its coating. Furthermore, we consider two cases: $\Omega_2$ with and without an air buffer region, as shown in Figure 3.1. The simulation setting for the reference problem, namely the single-domain FEM, is shown in Figure 3.2.

### 3.1.1 Iterative Convergence

First, we analyze the progression of simulation via electric field distribution and the residual of the iterative solver. The progression of field distribution with respect
Figure 3.2: Reference problem setting for the scattering of a dielectric-coated PEC sphere.

to iteration using setting (b) in Figure 3.1 is shown in Figure 3.3, where the simulation results of the first three iterations are presented. Moreover, Figure 3.4 provides the progression of electric field error distribution compared to the reference. From the results, we can clearly observe a well-established communication between the background and embedded subdomains, as well as a fast decrease of field errors through the iterative process.

Figure 3.5 gives the convergence of the GCR solver for the two $\Omega_2$ settings. In both cases, the proposed method exhibits a fast convergence and needs only a few iterations to converge for a relative residual equal to $10^{-8}$. Figure 3.5 also shows that embedded DDM with air buffer converges faster than that without air buffer.
Figure 3.3: Progression of electric field distribution in embedded DDM for the scattering of a dielectric coated PEC sphere: (a) first iteration; (b) second iteration; (c) third iteration.

Figure 3.4: Progression of electric field error distribution between embedded DDM and single-domain FEM for the scattering of a dielectric coated PEC sphere: (a) first iteration; (b) second iteration; (c) third iteration.
Next, we compare the converged results of embedded DDM with the results of single-domain FEM. Electric field distribution and bistatic radar-cross-section (RC-S) are depicted in Figures 3.6 and 3.7, respectively. In the figures, the results of embedded DDM agree reasonably well with the reference results. However, a slight difference exists between the results of embedded DDM with air buffer and that without air buffer. The higher accuracy and faster convergence (see Figure 3.5) of the air buffer case can be attributed to the extra overlapping in the air buffer region in $\Omega_2$, which allows for more information exchanged between the subdomains.

To further investigate the effect of the air buffer on the convergence, we employ a spherical air box for $\Omega_2$ and plot the change of the convergence behavior with respect to the air buffer size. As shown in Figure 3.8, the larger the overlapping buffer region is, the better the convergence rate becomes. This observation is closely
Figure 3.6: Field distributions on the air box and PEC sphere. (a) embedded D-DM with air buffer; (b) embedded DDM without air buffer; (c) single-domain FEM reference.
Figure 3.7: Comparison of bistatic RCS for the dielectric-coated PEC sphere between embedded DDM and single domain FEM.

Figure 3.8: The convergence behavior of the iterative solver regarding different air buffer sizes.
related to the convergence behavior of the Schwarz (overlapping) based DDM, whose the convergence rate increases with the size of overlapping regions [1, 2].

Therefore, buffer region would be useful in improving the accuracy and convergence of embedded DDM. Nevertheless, even without a buffer region, the convergence and accuracy of embedded DDM are already satisfactory.

3.1.2 Convergence Comparison with Nonoverlapping DDM

![Figure 3.9: Simulation settings for the subdomains with the air buffer region: (a) setup of embedded DDM subdomains; (b) setup of nonoverlapping DDM subdomains.](image)

Compared to existing nonoverlapping DDMs [8, 15, 16], the convergence of the proposed embedded DDM has an advantage. To demonstrate this, we still use the sphere scattering as the example for comparison. Two settings are studied: the first is the embedded subdomain with an air buffer, the second is the embedded subdomain without an air buffer. The corresponding nonoverlapping DDMs for comparison are shown in Figure 3.9 and Figure 3.10, respectively. Moreover, we check the convergences of two different types of nonoverlapping DDMs: the one with the Robin TC [8]
Figure 3.10: Simulation settings for the subdomains without the air buffer region: (a) setup of embedded DDM subdomains; (b) setup of nonoverlapping DDM subdomains.

and the one with the second order TC [15,16]. The same types of preconditioner and iterative solver are employed for all the DDM cases.

Figure 3.11: Convergence comparison between embedded DDM and nonoverlapping DDM for $\Omega_2$ with air buffer region.
Figure 3.12: Convergence comparison between embedded DDM and nonoverlapping DDM for $\Omega_2$ without air buffer region.

The results of convergence are shown in Figure 3.11 and Figure 3.12. We can observe that the convergence of embedded DDM is significantly better than the nonoverlapping DDM with the Robin TC, and slightly better than the nonoverlapping DDM with the second order TC.

3.1.3 Integral Equation Truncation

In Chapter 2, the embedded DDM is formulated with respect to ABC. However, ABC only provides a rough approximation to the radiation condition. Higher order of accuracy is still required when we need to deal with certain radiation and scattering problems. For such scenarios, the boundary element method (BEM) is preferred due to its correct representation of the exterior outer space. Consequently, we shall investigate the integral equation truncation for embedded DDM.
Herein, we combine embedded DDM with the FEM-BEM-DDM framework [77]. More specifically, the background $\Omega_1$ is still solved by using FEM. On $\Omega_1^{ext} = \mathbb{R}^3$ $\bar{\Omega}_1$ we define an exterior BEM domain, as shown in Figure 3.13. The two domains are separated by the closed surface $\partial \Omega_1$. Similar to FEM-DDM, we employ Robin TCs on $\partial \Omega_1$ to solve $\Omega_1$ and $\Omega_1^{ext}$. Meanwhile, $\Omega_1$ and $\Omega_2$ are coupled in the same way as previously established through embedded DDM. The simulation results are carried out and compared against the analytical Mie series solutions, as displayed in Figure 3.14. As expected, we observe that the integral equation truncation offers an accuracy improvement over ABC, and embedded DDM should work well with BEM.
Figure 3.14: The RCS results of the embedded DDM with integral equation truncated boundary and its comparison with ABC truncated boundary.
3.2 A Waveguide with PEC and Port Inside

In this section, we use a rectangular waveguide with specifically designed interior structures to validate our proposed formulation about PEC and port, and examine the h-convergence rate of embedded DDM. The geometrical details of the problem are plotted in Figure 3.15. The waveguide ports are both terminated with PMLs, and the port impedance of port 3 is $50 \, \Omega$. The operating frequency is $10 \, \text{GHz}$.

3.2.1 Verifications of the PEC and Port Coupling Sources

The waveguide is discretized using two subdomains: the background subdomain $\Omega_1$ and the interior subdomain $\Omega_2$. $\Omega_1$ is a simple waveguide while $\Omega_2$ contains the
PEC plates and port, as plotted in Figure 3.16. By checking the simulation results of reflection and transmission coefficients, we can verify whether or not the wave propagation in $\Omega_1$ correctly detects the existence of the PECs and port in $\Omega_2$.

The simulation is conducted with respect to three different cases of $\Omega_2$ settings. The first case is that $\Omega_2$ only contains PEC plates. Port 1 is the excitation and port 2 is the receiver. The simulation results are shown in Table 3.1. In the second case, $\Omega_2$ contains PEC plates as well as a passive port, port 3. Port 1 is the excitation, port 2 is the receiver, and port 3 can be viewed as a surface impedance. Table 3.2 summarizes the simulation results. The third case is similar to the second case except port 3 is now used as an active port. In this case, port 3 is the excitation, while port 1 and port 2 are the receivers. The simulation results are shown in Table 3.3.
### Table 3.1: S-Parameter Results for PEC Existing in the Waveguide.

<table>
<thead>
<tr>
<th>S Parameter</th>
<th>$S_{11}$</th>
<th>$S_{21}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Embedded DDM</td>
<td>$0.9463 \angle -119.3^\circ$</td>
<td>$0.3189 \angle 150.9^\circ$</td>
</tr>
<tr>
<td>Reference</td>
<td>$0.9477 \angle -119.4^\circ$</td>
<td>$0.3192 \angle 150.6^\circ$</td>
</tr>
</tbody>
</table>

### Table 3.2: S-Parameter Results for PEC and Passive Port Existing in the Waveguide.

<table>
<thead>
<tr>
<th>S Parameter</th>
<th>$S_{11}$</th>
<th>$S_{21}$</th>
<th>$S_{31}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Embedded DDM</td>
<td>$0.8656 \angle -148.4^\circ$</td>
<td>$0.2159 \angle -91.51^\circ$</td>
<td>$0.4335 \angle 178.0^\circ$</td>
</tr>
<tr>
<td>Reference</td>
<td>$0.8784 \angle -148.3^\circ$</td>
<td>$0.2076 \angle -88.82^\circ$</td>
<td>$0.4309 \angle 178.3^\circ$</td>
</tr>
</tbody>
</table>

### Table 3.3: S-Parameter Results for PEC and Active Port Existing in the Waveguide.

<table>
<thead>
<tr>
<th>S Parameter</th>
<th>$S_{33}$</th>
<th>$S_{13}$</th>
<th>$S_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Embedded DDM</td>
<td>$0.7835 \angle -22.25^\circ$</td>
<td>$0.4237 \angle 178.2^\circ$</td>
<td>$0.4238 \angle 178.2^\circ$</td>
</tr>
<tr>
<td>Reference</td>
<td>$0.7861 \angle -22.29^\circ$</td>
<td>$0.4309 \angle 178.3^\circ$</td>
<td>$0.4309 \angle 178.3^\circ$</td>
</tr>
</tbody>
</table>

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As can be seen, all the simulation cases in embedded DDM yield S-parameter results that agree well with the results of reference. Consequently, we can confirm the correctness of the surface current formulation for PEC and port aforementioned in Section 2.4.2.

### 3.2.2 H Convergence

Furthermore, we shall study the mesh refinement property of the method. To do so, we adopt three mesh sizes, 2 mm, 1 mm, and 0.5 mm, for both embedded DDM and sing-domain FEM. In embedded DDM, the background and embedded subdomains are discretized by using the same mesh sizes. For each set of mesh, we can computed the relative $L_2$ error between the overall field solutions of embedded DDM and those of single-domain FEM

$$
\text{Relative } L_2 \text{ Error } (h) = \frac{\| \mathbf{E}_{h,\text{Embedded,DDM}}^{h} - \mathbf{E}_{h,\text{FEM}}^{h} \|_2}{\| \mathbf{E}_{h,\text{FEM}}^{h} \|_2}
$$

where $\mathbf{E}_{h,\text{Embedded,DDM}}^{h}$ and $\mathbf{E}_{h,\text{FEM}}^{h}$, respectively, stand for the electric field solutions of embedded DDM and single-domain FEM with an average mesh size of $h$. The $L_2$ errors with respect to mesh sizes are plotted as “case 1” in Figure 3.17, where “0”, “1”, and “2” at the $x$ axis correspond to the mesh sizes of 2 mm, 1 mm, and 0.5 mm, respectively. Note we use the first-order basis in our FEM code, so the theoretical $h$-convergence rate of single-domain FEM is $h^2$. The convergence rate shown in the figure confirms that the proposed embedded DDM is of the same mesh-refinement quality as conventional FEM. Secondly, we use the mesh size 1 mm for the background, and refine the embedded meshes from 1 mm to 0.5 mm. The change of error is given as “case 2” in Figure 3.17. The convergence rate is $h^{1.6}$, which is a bit worse than the “case 1”. As for “case 3”, we keep the mesh size 2 mm for the background, while
refine the embedded meshes. The convergence rate is approximately $h^2$ when the embedded meshes are refined from 2 mm to 1 mm, and $h^{0.43}$ when the embedded meshes are refined from 1 mm to 0.5 mm.

According to the convergence study, in order to obtain the best accuracy convergence, the principle for mesh refinement is to refine the background and embedded meshes at the same time. The adaptive refinement for the embedded meshes can be done similarly to conventional FEM, while the refinement of the background mesh can be conducted by splitting the background tetrahedrons into smaller ones. If we only refine the meshes of the embedded structures, we may still have an accuracy improvement. However, it will not be as effective as refining both of the subdomain-s. Furthermore, if the background mesh is too coarse, the accuracy improvement of refining embedded meshes can be limited.
3.3 Surface Integration Scheme on $\Gamma_{21}$

In order to accurately model the geometrical details of the embedded objects, the meshes of $\Omega_2$ are usually dense. Therefore, it is convenient and efficient to choose a $\Gamma_{21}$ inside $\Gamma_{12}$. However, there are situations where $\Gamma_{21}$ touches or equals $\Gamma_{12}$, such as $\Omega_4$ in Figure 2.10. In our numerical experiment, we have found that directly using triangular Gaussian quadrature for the term $\left\langle \pi_r(v_1), \pi_{\times}^+\left(H_{(n-1)}^2\right) \right\rangle$ in (2.22) would give rise to non-smooth field distributions on $\Gamma_{21}$. When $\Gamma_{21} = \Gamma_{12}$, the non-smooth fields would propagate into $\Omega_1 \setminus \Omega_2$, thus decreasing the accuracy of the simulation results.

Figure 3.18: A capacitor mounted microstrip line and the corresponding simulation setup in embedded DDM.
Table 3.4: The S-Parameter Results of Different $\Gamma_{21}$ Settings for the Embedded Sub-domain of Capacitor.

<table>
<thead>
<tr>
<th>S-Parameter</th>
<th>$\Gamma_{21}$ inside $\Gamma_{12}$ Gaussian Quadrature</th>
<th>$\Gamma_{21} = \Gamma_{12}$ Gaussian Quadrature</th>
<th>$\Gamma_{21} = \Gamma_{12}$ Proposed</th>
<th>Single-Domain FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>S11</td>
<td>0.4890∠132.7°</td>
<td>0.5208∠123.3°</td>
<td>0.4842∠132.4°</td>
<td>0.4871∠133.0°</td>
</tr>
<tr>
<td>S21</td>
<td>0.5052∠-121.6°</td>
<td>0.4914∠-113.5°</td>
<td>0.5075∠-121.7°</td>
<td>0.5113∠-121.7°</td>
</tr>
</tbody>
</table>

Herein, we investigate a surface mount capacitor on a microstrip. As shown in Figure 3.18, the background subdomain is a microstrip line with an air box, and a capacitor is embedded into the background mesh. Moreover, buffer region is included in the embedded subdomain for the calculation of the surface currents on PECs. In this problem, $W = 3$ cm, $L_0 = 4$ cm, $H = 0.2$ cm, $L_1 = 1.67$ cm, $L_2 = 0.46$ cm, $w = 0.5$ cm, $h = 0.4$ cm, $\epsilon_r = 2$, and $\epsilon_r = 12$. For reference, we also solve the same problem with a conventional single-domain FEM solver.

First, we choose $\Gamma_{21}$ inside $\Gamma_{12}$ in $\Omega_2$ and carry out the simulation at 10 GHz by using the proposed method. $\Gamma_{12}$ is the boundary surface of $\Omega_2$ while $\Gamma_{21}$ is constructed by utilizing the mesh inside $\Omega_2$. The corresponding S-parameter results are listed in the second column in Table 3.4. Moreover, the field distribution results on $\Gamma_{12}$ is given in Figure 3.19a. Both results agree very well with the reference results of conventional FEM.

Next, we set $\Gamma_{21} = \Gamma_{12}$ and redo the simulation. As plotted in Figure 3.19c, non-smooth field distribution exists on $\Gamma_{12}$, which disagrees with single-domain FEM in
Figure 3.19e. Furthermore, the accuracy of the S-parameter results is also affected, as can be seen in the third column of Table 3.4.

Such phenomenon can be explained by the discontinuity of the testing function $\pi_\tau(v_1)$. Assuming we use the triangular Gaussian quadrature for the surface integrals on $\Gamma_{21}$ in (2.22), the corresponding formula can be written as

$$
\left\langle \pi_\tau(v_1), \pi_\times^+(H_2^{(n-1)}) \right\rangle_{\Gamma_{21}} = \sum_j \left[ \sum_i \left( \pi_\tau(v_{1,i}) \cdot \pi_\times^+(H_2^{(n-1)} \cdot \omega_i) \Delta_j \right) \right] (3.3)
$$

where $j$ is the index of the triangles on $\Gamma_{21}$, $\Delta_j$ is the area of the $j$-th triangle, $i$ is the index of Gaussian quadrature points in each triangle, and $\omega_i$ represents the weight associated with the $i$-th Gaussian point. $\pi_\times^+(H_2^{(n-1)})$ are calculated at the $i$-th sampling points of the same triangle. Therefore, they are continuous inside each triangle $j$. However, the testing functions $\pi_\tau(v_{1,i})$ can reside in different tetrahedrons when the triangle $j$ intersects more than one tetrahedron in $\Omega_1$. This would cause discontinuities in the testing functions. Such discontinuities would lead to non-smooth $\pi_\tau(v_{1,i}) \cdot \pi_\times^+(H_2^{(n-1)})$ on $\Gamma_{21}$.

To overcome the problem, we combine the triangular Gaussian quadrature integration with an h-refinement integration process, as shown in Figure 3.20. For the $j$-th triangle on $\Gamma_{21}$, we will check whether it is fully inside in a tetrahedron in $\Omega_1$ or not. If it is, the triangular Gaussian quadrature will be employed. Otherwise, the specific triangle is divided into four child triangles. Each child triangle is further subdivided into four child triangles unless it is completely contained in one tetrahedron. The h-refinement process will be performed iteratively until each child triangle is small enough or completely inside one tetrahedron in the background subdomain. Finally, we will compute the integration on the $j$-th triangle by summing the integrations of its child triangles.
Figure 3.19: The field distributions on $\Gamma_{12}$ and $\Gamma_{21}$: (a) $\Gamma_{21}$ inside $\Gamma_{12}$, Gaussian quadrature; (b) the $\Gamma_{21}$ inside $\Gamma_{12}$; (c) $\Gamma_{21} = \Gamma_{12}$, Gaussian quadrature; (d) $\Gamma_{21} = \Gamma_{12}$, Gaussian quadrature combined with h-refinement integration; (e) single-domain FEM.

After such modification, the agreement of embedded DDM and single-domain FEM can be improved when $\Gamma_{21} = \Gamma_{12}$. This can be observed in the field distribution in Figure 3.19d and the S-parameter results in the fourth column in Table 3.4.
Figure 3.20: The surface integration scheme on $\Gamma_{m1}$ for the embedded subdomain of capacitor.

3.4 Touched Interfaces Between Embedded Subdomains

In practical applications, the embedded subdomains may have touched surfaces or need to be physically connected to each other. If we treat the embedded subdomains separately and only construct the coupling sources between the background and embedded subdomains, discontinuous fields could emerge on the touched interface between the embedded subdomains.
To demonstrate this, we present an interconnect structure cut from a multilayer PCB, as shown in Figure 3.21a. The input signal is given at the bottom layer while the output port is established at the top layer. For simplicity, the ground vias are modelled as PEC sheets. In addition, $L = 13.42$ mm, $W = 7.36$ mm, and $H = 0.42$ mm. To investigate touched subdomains, we set the background subdomain $\Omega_1$ to be two ground planes and an air box. For the embedded subdomains, we divide the
Table 3.5: The S-Parameter Results of the Interconnect Structure.

<table>
<thead>
<tr>
<th>S-Parameter</th>
<th>Only Embedded DDM</th>
<th>Embedded DDM with Nonoverlapping TCs</th>
<th>Single-Domain FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>S11</td>
<td>0.6948∠167.1°</td>
<td>0.8155∠150.8°</td>
<td>0.8262∠151.0°</td>
</tr>
<tr>
<td>S21</td>
<td>0.3468∠52.48°</td>
<td>0.5035∠71.56°</td>
<td>0.4987∠72.03°</td>
</tr>
</tbody>
</table>

Figure 3.22: The field distributions of electric field magnitude on the top layer of the interconnect: (a) only embedded DDM; (b) embedded DDM with nonoverlapping TCs on the touched interfaces; (c) single-domain FEM.

interconnect into three parts Ω₂, Ω₃, and Ω₄, and embed them into the background Ω₁. The PEC structures in Ω₂, Ω₃, and Ω₄ are required to be physically touched.

We first apply the algorithm in Section 2.3 and Section 2.4 and conduct the simulation at 20 GHz. The S-parameter results are shown in the second column in Table 3.5, which exhibit a bad agreement with single-domain FEM. To figure out the cause of the disagreement, we further plot the field distribution results on the
top layer in Figure 3.22a. An abnormal field discontinuity is found on the touched interface $\Gamma_{34} (= \Gamma_{43})$ between $\Omega_3$ and $\Omega_4$.

The abnormal field on the touched interface is largely due to the mesh size difference between the background and embedded subdomains. Since the embedded subdomains are coupled into the background subdomain, they communicate indirectly in the background. In the simulation setup of this problem, the background subdomain does not see the geometrical details. As a consequence, the background mesh is coarser than the embedded subdomains. The accuracy of fields could decrease when we transfer them from the embedded subdomains into the background.

Our remedy is to let the embedded subdomains communicate directly on their touched surfaces. On top of the coupling sources in Section 2.2 and Section 2.4, we further introduce the nonoverlapping TCs [8, 12, 15, 16] on the touched interfaces between the embedded subdomains. Herein, we adopt the second order TC [15] due to its fast and stable convergence for both the propagating and evanescent modes in DDM.

Take $\Omega_3$ and $\Omega_4$ for example. Vector and scalar auxiliary variables $j_m$ and $\rho_m$, $m \in \{3, 4\}$ are introduced on $\Gamma_{34}$ and $\Gamma_{43}$

$$j_m := \frac{1}{k} \pi^+ \left( \frac{1}{\mu_{rm}} \nabla \times E_m \right)$$

$$\rho_m := \frac{1}{k} \nabla \cdot j_m = \frac{1}{k^2} \nabla \cdot \nabla \cdot \pi^+ \left( \frac{1}{\mu_{rm}} \nabla \times E_m \right)$$

$j_m$ and $\rho_m$ carry the physical meanings of the electric current and charge on the surfaces, respectively. With the help of the auxiliary variables, we state the TCs on $\Gamma_{34}$ and $\Gamma_{43}$ as

$$k j_3 + \alpha \pi^+ (E_3) + \beta \nabla \times \nabla \times \pi^+ (E_3) + \gamma k^2 \nabla \cdot \rho_3 = 54$$
\[-k\mathbf{j}_4 + \alpha \pi_\tau (\mathbf{E}_4) + \beta \nabla_\tau \times \nabla_\tau \times \pi_\tau (\mathbf{E}_4) - \gamma k^2 \nabla_\tau \rho_4 \tag{3.6}\]

\[k\mathbf{j}_4 + \alpha \pi_\tau (\mathbf{E}_4) + \beta \nabla_\tau \times \nabla_\tau \times \pi_\tau (\mathbf{E}_4) + \gamma k^2 \nabla_\tau \rho_4 =
-k\mathbf{j}_3 + \alpha \pi_\tau (\mathbf{E}_3) + \beta \nabla_\tau \times \nabla_\tau \times \pi_\tau (\mathbf{E}_3) - \gamma k^2 \nabla_\tau \rho_3 \tag{3.7}\]

where \(\alpha, \beta,\) and \(\gamma\) are complex coefficients. The nonoverlapping TCs shall offer the necessary continuities of the tangential electric and magnetic fields on the touched surfaces between two embedded subdomains. (3.6) will be tested by \(\pi_\tau (\mathbf{v}_3) \in H^{-1/2}(\text{curl}_\tau; \Gamma_{34})\) while (3.7) will be tested by \(\pi_\tau (\mathbf{v}_4) \in H^{-1/2}(\text{curl}_\tau; \Gamma_{43})\). Subsequently, coupling block matrices \(C_{34}\) and \(C_{43}\) need to be assembled and added into the system matrix in (2.25). The explicit forms of the block matrices can be found in [15].

After employing the second order TCs on \(\Gamma_{23}, \Gamma_{32}, \Gamma_{34},\) and \(\Gamma_{43}\), we rerun the simulation of the interconnect. Because the embedded subdomains have similar mesh densities, the field continuities on their touched interfaces are improved when they exchange fields directly, as depicted in Fig 3.22b. As a result, the accuracy of S11 and S21 is also enhanced, as displayed in the third column in Table 3.5.
Chapter 4: Applications of Embedded Domain Decomposition

The proposed embedded DDM is very attractive in practical designs and analyses, because it solves a problem from a different perspective compared to other existing CEM methods and provides several remarkable advantages. The first advantage comes from the nonconformal discretization between subdomains. By applying the strategy of embedded domain decomposition, complicated geometries can be decoupled into simpler ones, and meshes of good quality would be easier to obtain. Secondly, the method allows for completely nonconformal volume meshes between subdomains. As a result, the modification of one subdomain will hardly affect the discretization and matrix computation of another subdomain. This feature offers a high degree of flexibility in modeling and simulation, and facilitates adding or replacing objects in a problem in a straightforward manner. Furthermore, we can accomplish a physical design by introducing and investigating different embedded subdomains into a background subdomain. Lastly, existing meshes of complex geometries are reusable in the form of embedded subdomains. For example, if an antenna is already discretized and simulated in free space, we can reutilize the spent efforts by embedding the existing antenna meshes into another background subdomain like a mobile device, and analyzing the performance of the antenna in that environment without remeshing it.
Herein, it is also worth emphasizing that an overall full wave analysis consists of three steps: CAD modeling, mesh generation, and simulation. As pointed out in [78], for complicated industrial applications, more than half of the overall analysis time is attributed to the CAD modeling and mesh generation, rather than the simulation itself. Such estimation agrees very well with our experiences. Since we have to investigate many possible geometry combinations to finalize a design or analysis, a lot of time could be wasted on the associated repetitive modelings and discretizations. Therefore, the biggest benefit of embedded DDM is its flexibility in modelings and discretizations, which will significantly speed up the processes of repetitive simulations.

4.1 Electromagnetic Compatibility

Due to EM environments and electromagnetic compatibility (EMC) concerns, a radio frequency device design needs to be optimized/tested in a number of scenarios. For example, as displayed in Figure 4.1, we may first optimize the antenna performance in a cell phone for wireless communications. Afterwards, the cell phone performance and its the specific absorption rate (SAR) value near human bodies should be verified. Further simulation may be required for the EMI/EMC effects when extra devices, such as a nearby tablet, are considered. For such simulation procedure, embedded DDM would be very useful as it allow for nonconformal meshes in a problem domain.

4.1.1 Cell Phone Performance Near Human Bodies

As shown in Figure 4.2, we consider the simulation of a dual-band cell phone in the presence of human head and hand [79]. Particularly, we are interested in the
frequency band of the cell phone being used, and the impact of the cell phone on the human head and hand.

The geometrical details of the problem are shown in Figure 4.3 and the associated material properties are given in Table 4.1. A PCB and a planar inverted-F antenna (PIFA) are placed inside the cell phone. A surface current is impressed on the port of PIFA and used as the excitation of the problem. As can be seen, the problem is mainly comprised of four parts. Therefore, we discretize the problem into four subdomains: $\Omega_1$, $\Omega_2$, $\Omega_3$, and $\Omega_4$, as shown in Figure 4.4. $\Omega_1$ is made up of the human head and an air box in which the cellphone and human hand will be embedded. $\Omega_2$ contains the cover part of the cell phone while $\Omega_3$ contains the base part. The human hand is
Figure 4.2: (a) A hand-held cell phone near a human head; (b) The model of a cell phone.

Figure 4.3: Geometrical details of the cell phone components, human head, human hand, and the corresponding subdomain configurations.
included in $\Omega_4$. Moreover, we add air buffers for the embedded subdomains in order to improve convergence.

The CPU time for simulation is detailed in Table 4.2. As described in Chapter 2, we detect the locations of the Gaussian quadrature points and construct the coupling matrices between the subdomains, such as (2.12), in a pre-processing step. The data in Table 4.2 indicates that the pre-processing operations take a very small amount of time compared to the overall simulation time.

We first examine the S-parameter results of the antenna inside the cellphone. The magnitude and phase of S-parameter are shown in Figures 4.5 and 4.6, respectively. From the figures, we can observe a satisfactory match between the results of embedded DDM and those of conventional FEM.

Next, the field distribution generated by the proposed method is compared against reference at 900 MHz. Figure 4.7 shows the comparison of field distribution on the
Table 4.1: Material Properties for the Cell Phone Components, Human Head, and Hand.

<table>
<thead>
<tr>
<th>Materials &amp; Geometric Parts</th>
<th>Relative Permittivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>plastic, cell phone body, cover body</td>
<td>2.5</td>
</tr>
<tr>
<td>side/function/digit key, cover pad</td>
<td>3.5</td>
</tr>
<tr>
<td>LCD glass, LCD cover, key lighter</td>
<td>4.78</td>
</tr>
<tr>
<td>substrate</td>
<td>4.9</td>
</tr>
<tr>
<td>head skin</td>
<td>3.7 − j0.02</td>
</tr>
<tr>
<td>head fluid</td>
<td>40.8 − j14.9</td>
</tr>
<tr>
<td>hand</td>
<td>20 − j13.2</td>
</tr>
</tbody>
</table>

Table 4.2: CPU Time Summary of Embedded DDM for the Cell Phone Problem.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Location Detection</th>
<th>Coupling Matrix Construction</th>
<th>Rest Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time (hh:mm:ss)</td>
<td>00:00:35</td>
<td>00:02:22</td>
<td>01:51:27</td>
</tr>
</tbody>
</table>

Figure 4.5: Plot of the S-parameter magnitude of the antenna in the cell phone.
human head, hand, and cell phone. Figure 4.8 shows the comparison of field distribution on the battery, antenna, and PCB inside the cell phone. Both comparisons demonstrate a close agreement between embedded DDM and conventional FEM. In addition, the convergence results at 900 MHz are shown in Figure 4.9.

In practical engineering, electric performance of the cell phone may need to be evaluated in different hand gestures, distance and positions with respect to human head. Using conventional FEM, we need to re-mesh the problem whenever a geometrical change is made. However, by applying embedded DDM, we can simply move and rotate subdomains $\Omega_2$, $\Omega_3$, and $\Omega_4$ into desired positions without the necessity to modify their discretizations, owing to the nonconformal feature between the subdomains. Furthermore, diagonal block matrices representing the subdomains remain the same in the global system matrix (2.25). Only off-diagonal block matrices need
Figure 4.7: Field distribution on cell phone, human head, and hand: (a) results of embedded DDM; (b) results of reference.

Figure 4.8: Field distribution on PCB, antenna, and battery inside cellphone: (a) results of embedded DDM; (b) results of reference.
to be updated to reflect the spatial change. In this way, embedded DDM can avoid repetitive meshing compared to conventional FEM.

4.1.2 Electromagnetic Interference Between A Cell Phone and A Tablet

Without modifying the existing meshes, we can further embed a tablet subdomain $\Omega_5$ into the background $\Omega_1$, to compute the EM interference from the tablet to the cell phone, and SAR value in the human head due to the device radiations, as shown in Figure 4.10 and Figure 4.11. The tablet model is described in Figure 4.12, which is similar to the model used in [80].

Firstly, a surface current is introduced on the port of the antenna in the tablet. To evaluate the EM interference from the tablet to the cell phone, we calculate the received power at the port of the antenna in the cell phone. The EM interference
Figure 4.10: A hand-held cell phone near a human head and a tablet.

Figure 4.11: Embedded DDM setting for the cell phone, tablet and human bodies.

Figure 4.12: Geometrical illustration of the tablet model.
Figure 4.13: EM interference from the tablet to the cellphone and the accuracy comparison between embedded DDM and single-domain FEM.

then can be represented as the power ratio between the received power at the port of the cellphone to the transmitted power at the port of the tablet. The power ratios computed from embedded DDM and FEM reference are both plotted in Figure 4.13. From the figure, we can observe a satisfactory match between the results of embedded DDM and those of conventional FEM.

Next, we excite the antenna in the cellphone and the antenna in the tablet simultaneously, and compute the SAR distribution in the human head caused by the radiations of the devices. As shown in Figure 4.14 and Figure 4.15, the SAR distributions at 0.9 GHz and 2.4 GHz generated by embedded DDM closely resemble those generated by conventional FEM. It is well known that SAR value is critical in the design of mobile devices. If the SAR value of a device exceeds certain technical
Figure 4.14: SAR distribution in the human head at 0.9 GHz: (a) results of embedded DDM; (b) results of reference.

Figure 4.15: SAR distribution in the human head at 2.4 GHz: (a) results of embedded DDM; (b) results of reference.
specification, the device must be re-designed. Meanwhile, SAR value cannot be lowered arbitrarily because the transmitting power of cell phone/tablet has a minimum requirement. In order to achieve a good balance between the SAR value and the transmitting power, the design process of a mobile device could suffer from repetitive modeling and demand a great deal of simulation effort. In such design problem, embedded DDM would be helpful in improving efficiency.

### 4.2 Simulation of Complex Antenna Structures

In this section, we perform the simulation of a leaky wave antenna model. The model is built based on the descriptions in [81–83] and the problem is shown in Figure 4.16. A surface wave launcher [82] is used to excite a cylindrical TM surface-wave on the grounded dielectric slab and the planar conductor strips [81] are employed to transform the bounded surface wave to a radiating wave. The width of the conductor strip lines are modulated so as to provide the sinusoidal variations of effective permittivity along the longitudinal direction of propagation.

For such simulation/design task, the shapes of the conductor strips may need to be optimized repetitively. Therefore, embedded DDM would be a suitable simulation engine in that it can separate the modelings and discretizations of the changing geometrical parts. The simulation setup for this problem is presented in Figure 4.17, where the substrate, surface wave launcher, cable excitation and an air box constitute the background subdomain $\Omega_1$. The embedded subdomain $\Omega_2$ is modeled as the top conductor strips of the antenna as well as a buffer region. Here, impedance boundary condition (IBC) [84] is used for the simulation of the top conductors and the buffer
Figure 4.16: A leaky wave antenna model, including a cable excitation, a surface wave launcher, and width-modulated conductor strip lines.
Figure 4.17: The simulation setup of embedded DDM for the leaky wave antenna. The background includes the substrates, excitation, and an air box. The embedded subdomain includes the top conductors and a buffer region.
Figure 4.18: The generated meshes of the background and embedded subdomains for the leaky wave antenna.
Figure 4.19: Electric field distribution on the substrate surface of the background subdomain.

region is used for the calculation of the surface currents on IBC. Subsequently, we discretize the two subdomains independently and obtain their meshes in Figure 4.18.

First, we conduct the background simulation, and carry out the electric field distribution on the substrate surface of $\Omega_1$. The field distribution at 24.5 GHz is shown in Figure 4.19. Afterwards, we embed the meshes of the conductor strip lines. The positioning of the embedded meshes with respect to the background field
distribution are given in Figure 4.20. We can see that the strip lines are placed in such a way that the repetitions of the embedded structures closely conform to the periodic variations of the surface wave. Consequently, the antenna designers could benefit from embedded DDM by directly impressing and modulating geometries in a background subdomain and compared to the available field information in the background.

![Image: Figure 4.20: The positions of the conductor strips with respect to the field distribution results of the background subdomain.]

Next, we simulate $\Omega_1$ and $\Omega_2$ together and calculate the field distribution on the substrate surface. The electric field distribution is plotted in Figure 4.21 while the current distributions on the surface conductor strips are shown in Figure 4.22. A relative uniform phase front can be inspected, and the current amplitudes decrease as a function of distance to the radiating source of the surface wave launcher. This suggests that the EM properties of the leaky wave antenna is correctly captured by our proposed method.
Figure 4.21: Electric field distribution results on the substrate surface of the whole model.
Figure 4.22: Surface current distributions on the conductor strip lines.
Figure 4.23: The S-parameter simulation results of the leaky wave antenna and the comparison with the literature results.
Figure 4.24: The normalized far field pattern of the leaky wave antenna at different frequencies: (a) 22 GHz; (b) 24.5 GHz.
The simulation results of S11, and its comparison with the S11 reference in [81], are depicted in Figure 4.23. Reasonable agreements can be observed, which demonstrate the usefulness of embedded DDM in antenna simulation and design. The small discrepancy in Figure 4.23 between our simulation results and those from [81] can be attributed to the CAD model difference, due to the incomplete description of the geometric information in [81]. In addition, normalized far field patterns are plotted and the pointing angles of the main lobes are compared with measurements, in Figure 4.24 and Figure 4.25, respectively.

Figure 4.25: The main lobe pointing angles of the leaky wave antenna with respect to frequency.
4.3 Signal Integrity in Integrated Circuits

In the designs of PCBs and electronic packages, to meet certain technical requirements, it is often necessary to perform parameter optimizations for the shapes and materials of some components, identify the functionalities of certain structures, or add/replace a functional block. As a consequence, we have to conduct the simulations of an electronic system repetitively. Embedded DDM would be helpful in improving the efficiency.

4.3.1 Parameter Study of a Via Pair

![Diagram of a via pair between two ground planes](image)

Figure 4.26: A via pair between two ground planes.

In this example, we study the accuracy and convergence of the embedded DDM in parameter study. Figure 4.26 shows a via pair between two parallel plates, which acts as the transition between the top layer and bottom layer transmission lines. Port
Figure 4.27: Simulation settings of embedded DDM for the via pair: (a) the background subdomain of the two ground planes; (b) the embedded subdomain of the signal via; (c) the embedded subdomain of the ground via.

1 is the excitation of the problem while port 2 receives the signals. The characteristic impedance of each port is set to be $50 \, \Omega$.

In applying embedded DDM to solve this problem, we use five subdomains for discretization, as illustrated in Figure 4.27. The background subdomain includes the signal traces, ground planes, and an air box. The signal and ground vias, along with their buffer regions, are used as the embedded subdomains. The mesh of the signal/ground via will be created once and copied to the corresponding positions. Furthermore, we perform a parameter sweep of the via radius $r$ in the simulation.

The simulation results of S-parameters with respect to the differential and common modes are depicted in Figure 4.28 and Figure 4.29, respectively. For comparison, we solve the same problems with a standard single-domain FEM solver and the results are also plotted in the figures as the reference. From the results, we can observe a satisfactory match between the results of embedded DDM and those from the
Figure 4.28: The S-parameter results of the via pair: (a) SDD11; (b) SDD21.

reference. Figure 4.30 exhibits the convergence of the iterative process. In all the cases, the proposed method shows a fast convergence rate and requires only a few iterations to converge.

The CPU time during parameter sweep are shown in Table 4.3. Compared to conventional FEM, we only need to mesh the background subdomain once at \( r = 3 \). Afterwards, we can reuse the background mesh as well as its block matrix \( A_1 \) at \( r = 5 \) and \( r = 7 \). Only the geometries and meshes of the vias need to be modified during the parameter sweep. Hence, in parameter study, embedded DDM provides more convenience and efficiency than conventional single-domain FEM. Moreover, the meshes of the vias can be moved freely within the mesh of the background subdomain.
Figure 4.29: The S-parameter results of the via pair: (a) SCC11; (b) SCC21.

Figure 4.30: Iterative convergence of embedded DDM for the via pair simulation.
Table 4.3: Memory Usage and CPU Time Comparison Between Embedded DDM and Single-Domain FEM for the Via Pair During Parameter Sweep of the Via Radius.

<table>
<thead>
<tr>
<th>r (mil)</th>
<th>Method</th>
<th>DOFs</th>
<th>CPU Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Embedded DDM</td>
<td>284092</td>
<td>81s</td>
</tr>
<tr>
<td>3</td>
<td>FEM</td>
<td>302968</td>
<td>98s</td>
</tr>
<tr>
<td>5</td>
<td>Embedded DDM</td>
<td>276652</td>
<td>12s</td>
</tr>
<tr>
<td>5</td>
<td>FEM</td>
<td>296266</td>
<td>96s</td>
</tr>
<tr>
<td>7</td>
<td>Embedded DDM</td>
<td>277628</td>
<td>12s</td>
</tr>
<tr>
<td>7</td>
<td>FEM</td>
<td>296608</td>
<td>85s</td>
</tr>
</tbody>
</table>

Such features will give us great flexibility in meshing a PCB, and can be fully exploited in SI studies such as via pattern design and optimization [85].

4.3.2 Analysis of An IC Package

Consider a PCB-package-chip model shown in Figure 4.31. The dimensions of the model are shown in the figure and the material of the substrates is FR-4. Differential signals are excited at port 1 in the PCB part and received at the differential port 2 in the chip part. The model contains a variety of small geometrical entities such as via holes, soldering balls, and bonding wires. By employing embedded DDM, we can conveniently investigate the functionalities of different components in this model.

The geometry is decomposed into one background subdomain $\Omega_1$ and five embedded subdomains $\Omega_2$ to $\Omega_6$. The resulting subdomains are shown in Figure 4.32a and the corresponding meshes are displayed in Figure 4.32b. Here, we select the
embedded subdomains in accordance with their roles in signal transmission. For example, \( \Omega_2 \) is mainly responsible for carrying signals, \( \Omega_3 \) acts as the return path for the current from the chip to the package, while \( \Omega_4 \) to \( \Omega_6 \) connect the PCB ground with the package ground. Moreover, we include the buffer regions in the embedded subdomains in order to calculate the surface currents on the PECs. As can be seen in Figure 4.32b, the meshes between the subdomains are completely nonconformal. The nonconformity in the meshes will provide considerable freedom in modeling and simulating the problem. Particularly, we can put \( \Omega_2 \) to \( \Omega_6 \) successively into \( \Omega_1 \) to analyze their effects in signal transmission, conduct the parameter studies of \( \Omega_2 \) to \( \Omega_6 \) independently, or add more subdomains of vias into the model to improve signal integrity.

Figure 4.31: Geometrical details of the PCB-package-chip model.
From the above figures, it is also worth mentioning the difference between the meshing strategy of embedded DDM and that of nonoverlapping DDM. In nonoverlapping DDM, such as [17], geometries are divided into analogous subdomains. The application can be the ultimate performance check of a system. In contrast, embedded DDM selects subdomains according to the design process or their functionalities in a problem. Hence, embedded DDM is not proposed to compete with nonoverlapping DDM for multiscale problems. It is for scenarios where add-on components need to be included in the studies and design analyses.

Firstly, the subdomain containing differential signals is embedded into $\Omega_1$, and the initial transmission/reflection coefficients are computed. In the second step, we
add the traces and bonding wires that link the package ground to the chip ground, recalculated the S-parameters, and examine the changes. Finally, we include the via/solder-ball connections between the ground planes of the PCB and package.

The procedure is described in Figure 4.33, and the S-parameter results from each step are plotted in Figure 4.34. In addition, we give reference results for the simulation of the whole model, which are carried out in conventional FEM. As shown in Figure
Figure 4.34: The S-parameter results of the PCB-package-chip problem and their comparison with single-domain FEM: (a) SDD11; (b) SDD21.

4.34, the results of embedded DDM at the final step agree reasonably well with those of conventional FEM.

In Figure 4.34, we can also observe the discrepancies between the results of different steps, mostly at 22-30 GHz. This can be explained by the fact that at low frequencies the traces and bonding wires are electrically short. Therefore, the symmetry of the differential lines may not be of critical importance and few signals return through the ground. Under such circumstances, the continuity of the ground paths is relatively unimportant. However, when the frequency continues to increase, EM effects begin to dominate the behavior of the transmission lines. More currents will flow on the ground planes due to asymmetry differential traces, propagation latency
of signals, and 3-D EM coupling. Consequently, we see obvious effects at higher frequencies by connecting the grounds of PCB, packages, and chips in the step 2 and step 3. To demonstrate the 3-D EM phenomena, we further present the results of field distribution at 26.5 GHz in Figure 4.35.

In Table 4.4, we present the CPU time for each simulation step, and their comparisons with conventional FEM. Throughout the simulation process, each subdomain only needs to be meshed once. The numerical simulations of their different combinations will provide the desired information in design analyses. Furthermore, subdomain matrices $A_i$ (see equation (2.25)) as well as their factorizations can be reused when the other subdomains are added. For example, in the second step in Figure 4.33, we only need to compute $A_3$, $A_{13}$, and $A_{31}$, while the other block matrices, such as $A_1$ and $A_2$, are the same as in the first step. In this way, the impacts of different components to the signal integrity of the system can be efficiently evaluated.

<table>
<thead>
<tr>
<th>Steps</th>
<th>Method</th>
<th>DOFs</th>
<th>Modeling &amp; Meshing</th>
<th>CPU Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1</td>
<td>Embedded DDM</td>
<td>731274</td>
<td>2h ~ 3h</td>
<td>17m : 31s</td>
</tr>
<tr>
<td>Step 1</td>
<td>Single-Domain FEM</td>
<td>674958</td>
<td>2h ~ 3h</td>
<td>16m : 20s</td>
</tr>
<tr>
<td>Step 2</td>
<td>Embedded DDM</td>
<td>809352</td>
<td>10m ~ 20m</td>
<td>1m : 12s</td>
</tr>
<tr>
<td>Step 2</td>
<td>Single-Domain FEM</td>
<td>653722</td>
<td>1h ~ 2h</td>
<td>17m : 22s</td>
</tr>
<tr>
<td>Step 3</td>
<td>Embedded DDM</td>
<td>875560</td>
<td>10m ~ 20m</td>
<td>1m : 36s</td>
</tr>
<tr>
<td>Step 3</td>
<td>Single-Domain FEM</td>
<td>694808</td>
<td>1h ~ 2h</td>
<td>17m : 45s</td>
</tr>
</tbody>
</table>
Figure 4.35: The field distribution results of the PCB-package-chip problem at each simulation step: (a) top view; (b) side view.
Chapter 5: EM-Circuit Co-Simulation

In this chapter, we shall describe the integration of an EM solver with a general-purpose circuit simulator. DGTD is employed for EM simulation, while the circuit simulation is conducted with respect to SPICE or IBIS models. The EM and circuit solvers are connected through surface ports, with a self-consistent coupling scheme.

5.1 EM-Circuit Decomposition Method

Consider a microstrip line structure terminated with a device or circuit network. We use this system to illustrate how to address EM-circuit computation we are interested in. Firstly, The whole system is decomposed into two subsystems, one including the EM structure, the other containing the circuits, as shown in Figure 5.1.

Figure 5.1: Illustration of a mixed EM-circuit system.
The EM and circuit part will be solved by DGTD and a circuit simulator, respectively. Herein, we propose a self-consistent scheme to couple the two decomposed subsystems, that is to ensure

\[ V_{EM}^{AB} = V_{CKT}^{A'B'} \]  
\[ I_{EM}^{AB} = I_{CKT}^{A'B'} \] (5.1) (5.2)

through a circuit port, as shown in Figure 5.1. \( V_{EM}^{AB} \) stands for the voltage across the surface port, while \( I_{EM}^{AB} \) represents the current flowing on the planar surface in the EM structure. The voltage across the circuits is denoted by \( V_{CKT}^{A'B'} \), while the total current in the circuits is represented as \( I_{CKT}^{A'B'} \).

The coupling mechanism consists of two directions. From EM coupling to circuit, we compute the voltage across the circuit port and use it as the equivalent driving source for the circuit simulator. The current and voltage relation for circuit network is denoted as (5.3). From circuit coupling to EM, we take the current calculated from the circuit solver and use it as the equivalent current source for full-wave simulation. Afterwards, the voltage on the circuit port is calculated from full-wave simulation, and we define this process as (5.4). The two processes are demonstrated in Figure 5.2.

\[ I_{CKT} = f(V_{CKT}) \]  
\[ V_{EM} = g(I_{EM}) \] (5.3) (5.4)

This coupling mechanism alone, however, can only ensure (5.2) by substituting \( I_{CKT} \) as \( I_{EM} \) for (5.4). However, (5.1) is not promised. Note in [51], similarly, (5.2) is ensured but not (5.1). This is the reason and where we add the self-consistent scheme in.
To illustrate our point, we apply one of the self-consistent conditions (5.2), and obtain

\[ V_{EM} = g(I_{EM}) = g(I_{CKT}) = g(f(V_{CKT})) \]  

(5.5)

Here, \( f \) is the general function that describes the current-voltage relations for arbitrary circuit network or semiconductor devices, thus it can be either linear or nonlinear; function \( g \) links the current and voltage in the full-wave EM system, and it is linear. Information exchange between the EM and circuits flows as \( V_{CKT} \xrightarrow{I} I \xrightarrow{g} V_{EM} \).

Note that (5.1) requires \( V_{CKT} \) and \( V_{EM} \) to be consistent. If only (5.2) is ensured, the difference of \( V_{CKT} \) and \( V_{EM} \) could become large after such information flowing with a highly nonlinear \( f \). The difference may result in nonphysical or unstable solutions as time marches on. This problem could be avoided by choose a small enough time step to keep the difference of \( V_{CKT} \) and \( V_{EM} \) sufficiently small. Nevertheless, that degree of “small” is not easy to control and it may cost too much computational resources.
As a result, (5.1) should be ensured throughout co-simulation. Generally speaking, \( gf = 1 \) is not necessarily true. However, we can find certain \( V_{\text{CKT}} \) and \( V_{\text{EM}} \) pairs, satisfying both (5.1) and (5.5) with an acceptable tolerance. Subsequently, we have the following self-consistent looping process:

- Start from the \( k \)-th iteration and do the simulation of \( V_{\text{CKT}}^k \rightarrow I_{\text{CKT}}^k \rightarrow I_{\text{EM}}^k \rightarrow V_{\text{EM}}^k \).

- Compare \( V_{\text{CKT}}^k \) with \( V_{\text{EM}}^k \). If their difference is smaller than a predefined tolerance, stop looping. Otherwise, add \( \Delta V \) to \( V_{\text{CKT}}^k \)

\[
V_{\text{CKT}}^{k+1} = V_{\text{CKT}}^k + \Delta V \tag{5.6}
\]

- To find \( V_{\text{CKT}}^{k+1} = V_{\text{EM}}^{k+1} = g(f(V_{\text{CKT}}^{k+1})) \), apply the Taylor’s expansion of the function \( V_{\text{EM}} = g(f(V_{\text{CKT}}^k)) \) at \( V_{\text{CKT}}^k \), ignore the second and higher order terms, and we obtain

\[
V_{\text{CKT}}^{k+1} = g(f(V_{\text{CKT}}^k)) = g(f(V_{\text{CKT}}^k)) + \frac{\partial gf}{\partial V}|_{V_{\text{CKT}}^k} \Delta V \tag{5.7}
\]

Since \( V_{\text{EM}}^k = g(f(V_{\text{CKT}}^k)) \), associating with (5.6), we have

\[
\Delta V = \frac{V_{\text{EM}}^k - V_{\text{CKT}}^k}{\frac{\partial gf}{\partial V}|_{V_{\text{CKT}}^k} - 1} \tag{5.8}
\]

- \( V_{\text{CKT}}^{k+1} \) is calculated as (5.6), and used as the input voltage to the circuit network for the next iteration, until convergence is achieved.

As can be seen from above, the derived looping process is similar to the Newton-Raphson method [86]. And here the initial guess is set to be \( V_{\text{CKT}}^0 \). Therefore, the looping method should also share the property of the Newton-Raphson method that provides a fast convergence rate for the iterations.
5.2 Simulation of the EM Part

5.2.1 Interior Penalty DGTD Formulation

The EM part is described by the time-dependent Maxwell’s equations in bounded three-dimensional domain $\Omega$ as,

\begin{align*}
\nabla \times \mathbf{E} &= -\mu \frac{\partial \mathbf{H}}{\partial t} \\
\nabla \times \mathbf{H} &= \epsilon \frac{\partial \mathbf{E}}{\partial t}
\end{align*}

(5.9)

where the electric permittivity $\epsilon(\mathbf{r})$ and the magnetic permeability $\mu(\mathbf{r})$ vary in the space $\Omega$.

In the computational domain of interest $\Omega$, let $\mathcal{T}_h$ be the discretization of $\Omega$ into tetrahedral elements $\{K_i\}$. We denote the set of all faces as $\mathcal{F}_h = \mathcal{F}_h^I \cup \mathcal{F}_h^B$, where $\mathcal{F}_h^I$ represents the set of interior faces between adjacent elements of $\mathcal{T}_h$, $\partial K_i \cap \partial K_j$, and $\mathcal{F}_h^B$ the set of boundary faces $\partial K_i \cap \partial \Omega$.

Following the procedure presented in [47,54,56], we can derive the interior penalty DGTD formulation for the first order Maxwell’s equations in time domain. Firstly, the finite-dimensional discrete space is introduced as $V_h^p = \{ \mathbf{v} \in [L^2(\Omega)]^3 : \mathbf{v}|_K \in [P^p(K)]^3, \forall K \in \mathcal{T}_h \}$, where $L^2(\Omega)$ is the space of square-integrable vector fields in domain $\Omega$, and $P^p(K)$ is the polynomial space of order $p$ in element $K$. Then we can state the DGTD formulation as:

Find $(\mathbf{E}, \mathbf{H}) \in V_h^p \times V_h^p$ such that

\[
\int_{\Omega} \mathbf{w} \cdot \left( \nabla \times \mathbf{E} + \mu \frac{\partial \mathbf{H}}{\partial t} \right) dV - \int_{\Omega} \mathbf{v} \cdot \left( \nabla \times \mathbf{H} + \epsilon \frac{\partial \mathbf{E}}{\partial t} \right) dV \\
+ \int_{\mathcal{F}_h} \{\mathbf{v}\} \cdot [\mathbf{H}]_\gamma dS - \int_{\mathcal{F}_h} \{\mathbf{w}\} \cdot [\mathbf{E}]_\gamma dS \\
+ e \int_{\mathcal{F}_h} [\mathbf{v}]_\pi \cdot [\mathbf{E}]_\pi dS + f \int_{\mathcal{F}_h} [\mathbf{w}]_\pi \cdot [\mathbf{H}]_\pi dS = 0,
\]
∀ (v, w) ∈ \( V_h^p \times V_h^p \). \hspace{1cm} (5.10)

where the notations are defined as follows,

\[
\begin{align*}
on \mathcal{F}_h^l \quad \left\{ \begin{array}{l}
\{ \{u\} \} = \left( \pi_\tau(u_i) + \pi_\tau(u_j) \right)/2 \\
[\mathbf{u}]_x = \pi_x(u_i) + \pi_x(u_j) \\
[\mathbf{u}]_\pi = \pi_\tau(u_i) - \pi_\tau(u_j)
\end{array} \right. \\
on \mathcal{F}_h^B \quad \left\{ \begin{array}{l}
\{ \{u\} \} = \pi_\tau(u) \\
[\mathbf{u}]_x = \pi_x(u) \\
[\mathbf{u}]_\pi = \pi_\tau(u_i)
\end{array} \right. \hspace{1cm} (5.11, 5.12)
\]

For the value of \( e \) and \( f \), we choose \( e = \frac{1}{2Z} \) and \( f = \frac{1}{2Y} \) with \( Z = \frac{1}{2}(\sqrt{\mu_i/\epsilon_i} + \sqrt{\mu_j/\epsilon_j}) \) and \( Y = \frac{1}{2}(\sqrt{\epsilon_i/\mu_i} + \sqrt{\epsilon_j/\mu_j}) \), to obtain an upwind numerical flux with an optimal convergence rate \( O(h^{p+1}) \) [55].

**Time Discretization**

Assume the number of DOFs in element \( K_i \) is \( d_i \), we can express the local electric and magnetic fields as \( E_h^{(i)}(r, t) = \sum d_i e_{in}(t)v_{in}(r) \) and \( H_h^{(i)}(r, t) = \sum d_i h_{in}(t)w_{in}(r) \) in terms of basis functions \( v, w \), where \( e_{in}(t) \) and \( h_{in}(t) \) are the time dependent coefficients for the basis functions. By separating the \( v, w \) testing in (5.10), we can build a local semi-discrete system within element \( K_i \) as

\[
M_e \frac{\partial \mathbf{e}_i}{\partial t} = \mathbf{S}_e \mathbf{h}_i - \mathbf{F}^{ij}_e \mathbf{h}_j + e \mathbf{P}^{ij}_e \mathbf{e}_j
\]

\[
-\mathbf{F}^{ij}_e \mathbf{h}_j + e \mathbf{P}^{ij}_e \mathbf{e}_j
\]

\[
M_\mu \frac{\partial \mathbf{h}_i}{\partial t} = -\mathbf{S}_h \mathbf{e}_i + \mathbf{F}^{ij}_h \mathbf{e}_j + f \mathbf{P}^{ij}_h \mathbf{h}_i
\]

\[
+\mathbf{F}^{ij}_h \mathbf{e}_j + f \mathbf{P}^{ij}_h \mathbf{h}_j
\]

where \( \mathbf{e}_i(t) \) and \( \mathbf{h}_i(t) \) are the time dependent coefficient vectors of the electric and magnetic fields, respectively. \( j \) is the index of the neighboring elements of element \( i \).
The local matrices are expressed as

\[
\begin{align*}
(M^e_i)_{nm} &= \int_{K_i} v_{in} \cdot \epsilon_i v_{im} dV & (M^e_i)_{nm} &= \int_{K_i} w_{in} \cdot \mu_i w_{im} dV \\
(S^e_i)_{nm} &= \int_{K_i} v_{in} \cdot \nabla \times w_{im} dV & (S^e_i)_{nm} &= \int_{K_i} w_{in} \cdot \nabla \times v_{im} dV \\
(F^{ii}_e)_{nm} &= \frac{1}{2} \int_{F_h^e} \pi_r(v_{in}) \cdot \gamma_r(w_{im}) dS & (F^{ii}_h)_{nm} &= \frac{1}{2} \int_{F_h^e} \pi_r(w_{in}) \cdot \gamma_r(v_{im}) dS \\
(F^{ij}_e)_{nm} &= \frac{1}{2} \int_{F_h^e} \pi_r(v_{in}) \cdot \pi_r(v_{jm}) dS & (F^{ij}_h)_{nm} &= \frac{1}{2} \int_{F_h^e} \pi_r(w_{in}) \cdot \pi_r(w_{jm}) dS \\
(P^{ii}_e)_{nm} &= \int_{F_h^e} \pi_r(v_{in}) \cdot \pi_r(v_{im}) dS & (P^{ii}_h)_{nm} &= \int_{F_h^e} \pi_r(w_{in}) \cdot \pi_r(w_{im}) dS \\
(P^{ij}_e)_{nm} &= \int_{F_h^e} \pi_r(v_{in}) \cdot \pi_r(v_{jm}) dS & (P^{ij}_h)_{nm} &= \int_{F_h^e} \pi_r(w_{in}) \cdot \pi_r(w_{jm}) dS
\end{align*}
\]

The first-order time derivatives in the resulting differential equations (5.13) can be discretized by using central difference approximation with second order accuracy. The electric field unknowns are evaluated at \( t^n = n\delta t \) while the magnetic field unknowns are evaluated at \( t^{n+1/2} = (n + 1/2)\delta t \). For the two penalty terms arising from upwind flux formulation, we apply a backward approximation as

\[
\begin{align*}
ed^{n+1/2} &\approx \ed^n \\
h^{n+1/2} &\approx h^n
\end{align*}
\]

for achieving an explicit time marching scheme. As a result, the fully discretized local system of equations can be expressed as

\[
\begin{align*}
M^e_i e^{n+1}_i &= (M^e_i + e\delta t P^{ii}_e) e^n_i + \delta t (S^e_i - F^{ii}_e) h^{n+1/2}_i - \delta t F^{ij}_e h^{n+1/2}_j + e\delta t P^{ij}_e e^n_j \\
M^\mu_i h^{n+3/2}_i &= (M^\mu_i + f\delta t P^{ii}_h) h^{n+1/2}_i + \delta t (-S^h_i + F^{ii}_h) e^{n+1}_i + \delta t F^{ij}_h e^{n+1}_j + f\delta t P^{ij}_h h^{n+1/2}_j
\end{align*}
\]

In addition, local time stepping technique is employed to reduce the computational time for multiscale structures and the stability analysis is the same as mentioned in [47].
5.2.2 Circuit Coupling to DGTD

Regarding the full-wave simulation of (5.4), modification is needed for elements in the vicinity of the circuit port. Retrieving the DGTD work on lumped elements [47], in general we model circuit ports as planar impedance surfaces, as shown in Figure 5.3. Compared to wavelength, the port dimension is usually much smaller. Hence, the current densities can be assumed to be constant on the surface. Without loss of generosity, we can address two elements \( K_i, K_j \) that share a face \( \partial K_i \cap \partial K_j \) on the surface \( \Gamma_{\text{CKT}} \) as shown in Figure 5.3.

![Geometrical illustration of the circuit port \( \Gamma_{\text{CKT}} \), where the current density is obtained from the circuit part.](image)

According to the boundary conditions of the electric and magnetic fields, the relationships on the port \( \Gamma_{\text{CKT}} \) can be stated as,

\[
\mathbf{n}_i \times \mathbf{H}_i + \mathbf{n}_j \times \mathbf{H}_j = J_{\text{CKT}} = \frac{I_{\text{CKT}}}{w} \quad (5.17)
\]
\[ \hat{n}_i \times \mathbf{E}_i + \hat{n}_j \times \mathbf{E}_j = 0 \quad (5.18) \]

The magnetic field relationship (5.17) is used to represent the electric currents from the circuits. Meanwhile, the electric fields need to be tangentially continuous across the surface port (5.18) since no magnetic currents exist on it. Consequently, we can enforce the two relationships weakly through the interior penalty approach. The corresponding residuals can be written as,

\[
\text{Residuals} \quad \text{Function Space}
\]

\[
\mathbf{R}^{(1)}_{\Gamma_{\text{CKT}}} = [\mathbf{H}] \times - J_{\text{CKT}} \quad \in \mathbf{H}^{-1/2}(\text{div}_\tau; \Gamma_{\text{CKT}}) \quad (5.19)
\]

\[
\mathbf{R}^{(2)}_{\Gamma_{\text{CKT}}} = [\mathbf{E}] \times \in \mathbf{H}^{-1/2}(\text{div}_\tau; \Gamma_{\text{CKT}}) \quad (5.20)
\]

As shown in [47], the residuals \( \mathbf{R}^{(1)}_{\Gamma_{\text{CKT}}} \) and \( \mathbf{R}^{(2)}_{\Gamma_{\text{CKT}}} \) represent the surface electric and magnetic error currents, respectively. According to the dual pairing principle of forming reaction integrals, \( \mathbf{R}^{(1)}_{\Gamma_{\text{CKT}}} \) should be tested with a surface \( \mathbf{E} \) to form the energy density \( \mathbf{E} \cdot \mathbf{J}^{\text{err}} \), thereby we adopt \( \pi_\tau(\mathbf{v}) \), which lies in the space \( \mathbf{H}^{-1/2}(\text{curl}_\tau; \Gamma_{\text{CKT}}) \), as the testing function for it. Similarly, \( \mathbf{R}^{(2)}_{\Gamma_{\text{CKT}}} \) should be tested with surface \( \mathbf{H} \) and we choose the testing functions as \( \pi_\tau(\mathbf{w}) \).

With respect to the above analysis, we can replace the interior penalty formulation of (5.10) for the elements that share the faces on the circuit port \( \Gamma_{\text{CKT}} \), as follows,

\[
\int_{\Gamma} \mathbf{w} \cdot \left( \nabla \times \mathbf{E} + \mu \frac{\partial \mathbf{H}}{\partial t} \right) dV - \int_{\Gamma} \mathbf{v} \cdot \left( \nabla \times \mathbf{H} + \epsilon \frac{\partial \mathbf{E}}{\partial t} \right) dV + \int_{\mathcal{F}_h} \{\mathbf{v}\} \cdot ([\mathbf{H}]_\gamma - J_{\text{CKT}}) dS - \int_{\mathcal{F}_h} \{\mathbf{w}\} \cdot [\mathbf{E}]_\gamma dS = 0 \quad (5.21)
\]

By separating the \( \mathbf{w} \) and \( \mathbf{v} \) testings, we can further obtain local the semi-discrete equations for element \( K_i \) as

\[
\mathbf{M}_e \frac{\partial \mathbf{e}_i}{\partial t} = \mathbf{S}_e \mathbf{h}_i - \mathbf{F}_e^{ii} \mathbf{h}_i + \mathbf{B}_e^{i} J_{\text{CKT}} - \mathbf{F}_e^{ij} \mathbf{h}_j \quad (5.22)
\]
\[
\begin{align*}
M_\mu \frac{\partial h_i}{\partial t} &= -S_h e_i + F^{ii}_h e_i + F^{ij}_h e_j \\
\end{align*}
\] (5.23)

where \((B'_{\mu})_n = \frac{1}{2} \int_{F_h} \pi_r (v_{in}) \cdot \hat{l}\) and \(\hat{l}\) denotes the unit vector along the length direction of the port. Likewise as (5.15), we apply the central difference approximation to time derivatives and evaluate \(J_{\text{CKT}}\) at \(t^{n+\frac{1}{2}} = (n+\frac{1}{2})\delta t\). The resulting local time-dependent update equations can then be written as

\[
\begin{align*}
M_i e_i^{n+1} &= M_i e_i^n + \delta t (S_i^{ii} - F^{ii}_h) h_i^{n+\frac{1}{2}} + B_j J_{\text{CKT}}^{j n+\frac{1}{2}} - \delta t F^{ij}_h h_j^{n+\frac{1}{2}} \\
M_i h_i^{n+\frac{3}{2}} &= M_i h_i^{n+\frac{1}{2}} + \delta t (-S_i^{ii} + F^{ii}_h) e_i^{n+1} + \delta t F^{ij}_h e_j^{n+1} \\
\end{align*}
\] (5.24)

After the EM simulation completes, we can compute the voltage across the surface port in an average sense,

\[
V_{\text{EM}} = \frac{1}{w} \int_0^w \int_0^l E(x) \cdot \hat{l} dx^2 = \frac{1}{w} \int_0^w V(x) dx = \frac{1}{w} \sum_{i=1}^N V(x_i) \text{wgt}(x_i) \\
\] (5.26)

where \(\int_0^w V(x) dx\) is carried out by employing Gaussian quadrature integration [86]. Moreover, \(N\) is the number of Gaussian quadrature points, \(\text{wgt}(x_i)\) is the weight corresponding to the \(i\)-th point.

### 5.3 Simulation of the Circuit Part

Herein, we investigate the circuit simulation corresponding to two types of circuit models: SPICE and IBIS.

#### 5.3.1 EM Coupling to SPICE Model

For circuits based on the SPICE model, we adopt Ngspice [63] as the simulation program. With regard to (5.3), we execute Ngspice for circuits until a certain time step, save the continuous quantities in the circuits like voltages/currents/charges/powers,
and let it wait for running command. After DGTD produces a new value of voltage, we change the parameters in the circuits, apply the stored quantities of circuits as initial conditions, and resume the circuit simulation from the previous time step.

To clarify the implementation process, we assume the simulation results of EM and circuit systems are known at time $t^n = n\delta t$, which should include $V_{\text{CKT}}^n$, $v_{\text{cap}}^n$, $i_{\text{ind}}^n$, and $V_{\text{CKT}}^{n+1}$. $v_{\text{cap}}^n$ denotes the voltages across the capacitors while $i_{\text{ind}}^n$ represents the currents in the inductors at $t^n = n\delta t$. These quantities are the input to drive the circuits in Ngspice, which are saved from the simulation results of DGTD from $t^n$ to $t^{n+1}$ and the simulation results of Ngspice from $t^{n-1}$ to $t^n$. More specifically, we can write (5.3) with all the input/output variables as

$$(I_{\text{CKT}}^{n+\frac{1}{2}}, v_{\text{cap}}^{n+1}, i_{\text{ind}}^{n+1}) = f_{\text{SPICE}}(V_{\text{CKT}}^n, V_{\text{CKT}}^{n+1}, v_{\text{cap}}^n, i_{\text{ind}}^n)$$

from $t^n$ to $t^{n+1}$. The voltage pair $V_{\text{CKT}}^n, V_{\text{CKT}}^{n+1}$ are employed to construct a piecewise linear voltage pulse in Ngspice with $V_{\text{CKT}}^n$ at $t^n$ and $V_{\text{CKT}}^{n+1}$ at $t^{n+1}$, in order to drive the circuit subsystem. $v_{\text{cap}}^{n+1}$ and $i_{\text{ind}}^{n+1}$ are saved and will be used as the initial conditions for the simulation of the next time step, namely from $t^{n+1}$ to $t^{n+2}$. Note for a multi-port circuit network, multiple voltages sources should be built, with multiple port currents coupling back to DGTD. A typical input file in SPICE is demonstrated in Figure 5.4.

As pointed out by [50], there are scenarios where only network information such as S/Y-parameters is known for circuits. These situations require DGTD to solve with circuit network represented by admittance matrix. Note the proposed DGTD-SPICE method intrinsically has this feature as well. An insightful discussion on SPICE-compatible representations of S-parameter matrices (yet not the only way) can be
found in [87]. With the S/Y-parameters provided or tabular S/Y-parameters measured of real-life multi-port circuit network or devices, we can employ the rational approximation method first, like on vector fitting basis [88, 89], and then write the netlists for the corresponding S/Y-parameter or admittance matrices. More specifically, either S/Y-parameter matrices or admittance matrices can be represented in SPICE with a combination of E-elements (voltage-dependent voltage sources), F-elements (current-dependent current sources), G-elements (voltage-dependent current sources), and H-elements (current-dependent voltage sources), along with the “LAPLACE” option in HSPICE [62] or “XSPICE” option in Ngspice [63].

### 5.3.2 EM Coupling to IBIS Model

In order to simulate a system level PCB, all the components on the board need to be modeled. Unfortunately, the SPICE models of many digital chips are not readily
Figure 5.5: The circuit components in the IBIS models: (a) an input buffer; (b) an output buffer.

available from semiconductor vendors due to intellectual property protections. As a result, behavioral modeling is evolved. The IBIS model [64–69] is a widely accepted standard for the behavioral specification of the input/output characteristics of digital circuits. It is developed for IP protection concerns and to simplify the IC simulations while maintaining an acceptable level of accuracy.

The IBIS model is in the form of an ASCII file, and is generated from the SPICE simulation of an integrated circuit or from measurements in the laboratory. It mainly models the system-level PCB behavior, specifically the interactions between the outside PCB and the chip’s digital I/O buffers. There are two types of IBIS model: the input buffer model and the output buffer model, as shown in Figure 5.5. Both models include the characteristics of the package parasitics ($R_{pkg}$, $L_{pkg}$, and $C_{pkg}$), the silicon input capacitance ($C_{comp}$) for the pin and the current-voltage tables of the ESD protection diodes. Furthermore, the output buffer model contains the DC information of the pull-up/pull-down transistors in the form of current-voltage tables, and the AC behaviors of the transistors in the form of voltage-time tables.
Figure 5.6: The equivalent transient circuit simulation of the IBIS models: (a) the IBIS input buffer; (b) the IBIS output buffer.

To simulate the IBIS circuits together with DGTD, we first construct the equivalent transient models from the IBIS file. Herein, we take the IBIS output model for example. The IBIS input model can be addressed in a very similar way.

As shown in Figure 5.6, \( C_{comp} \) consists of the capacitances of the transistors, on-die interconnect, and die pad. It is extracted by connecting the circuit to an AC voltage source at the I/O pad so that all the contributors to the capacitance can be captured. The current-voltage tables are constructed by connecting the circuit output to an independent voltage source. The voltage source is swept across a range of values and the currents flowing into the pad are recorded in different logical states. Subsequently, four current-voltage tables are generated, corresponding to the DC behaviors of pull-up, pull-down, power clamp, and ground clamp devices. The voltage-time tables \( V(t) \) of the IBIS model are generated when the circuits are driving into a test load without package parasitics, as described in Figure 5.7. The rising and falling edges of the buffers (‘0’ to ‘1’ and ‘1’ to ‘0’) are simulated/measured with respect to two different loading voltages. As a result, four \( V(t) \) tables are generated.
Before the simulation of the IBIS model can be conducted, we need to describe the dynamic switching behaviors of the pull-up and pull-down devices during the transitions of logical states. Therefore, we introduce time dependent multipliers \( K_{u}(t) \) and \( K_{d}(t) \) [65] to the current sources \( I_{pu}(V) \) and \( I_{pd}(V) \), respectively. There are four time \( K_{u}(t)/K_{d}(t) \) multipliers in total, one \( K_{u}(t) \) and \( K_{d}(t) \) pair related to the rising edge of signals, one \( K_{u}(t) \) and \( K_{d}(t) \) pair related to the falling edge of signals. Because we have four \( V(t) \) tables simulated or measured in a typical IBIS model, the \( K_{u}(t) \) and \( K_{d}(t) \) multipliers can be obtained by solving the circuit equations of Figure 5.7 in a matrix form [66].

More specifically, we detail the transition behaviors of the multipliers \( K_{u}(t) \) and \( K_{d}(t) \), the pull-up device (represented as voltage controlled current source \( I_{pu}(V) \)), and the pull-down device (represented as \( I_{pd}(V) \)), when a rectangular pulse is sent into an IBIS model, as shown in Figures 5.8 and 5.9. Here, \( V_{dd} \) is the power supply voltage and we use \( V_{dd}/2 \) as the threshold for logical transitions.

- From \( T_{0} \) to \( T_{1} \), the input signal is smaller than \( V_{dd}/2 \), therefore \( I_{pu}(V) \) is off and \( I_{pd}(V) \) is on, to represent ‘0’.
Figure 5.8: The transitions of the current sources in the IBIS output buffer during signal changes and the interface with DGTD.
Figure 5.9: The transitions of the current sources in the IBIS output buffer during signal changes and the interface with DGTD.

- At $T_1$, the input signal changes across $V_{dd}/2$, and the two transistors switch from steady state to transition state. At transition state, pull up transistor (Ipu) changes from off to on, so $K_u(t)$ changes from 0 to 1. Meanwhile, pull down transistor (Ipd) changes from on to off, so $K_d(t)$ changes from 1 to 0. The time-dependent coefficients $K_u(t)$ and $K_d(t)$ represent the transition status of the transistors. At $T_2$, the transistors go to the steady state of logical ‘1’, Ipu turns on and Ipd turns off completely. The transit time $T_2 - T_1$ can be extracted from the IBIS file.

- From $T_2$ to $T_3$, the input signal is larger than $V_{dd}/2$, therefore $Ipu(V)$ is on and $Ipd(V)$ is off, to represent ‘1’.

- At $T_3$, the input signal changes across $V_{dd}/2$, and the two transistors switch from steady state to transition state. At transition state, pull up transistor (Ipu) changes from on to off, so $K_u(t)$ changes from 1 to 0. Meanwhile, pull down transistor (Ipd) changes from off to on, so $K_d(t)$ changes from 0 to 1. At
Figure 5.10: The block diagram of the assembled IBIS model with input and output buffers.

\[ T_4 \], the transistors go to the steady state of '0', Ipu turns off and Ipd turns on completely. The transit time \( T_4 - T_3 \) can be extracted from the IBIS file.

- From \( T_4 \) to \( T_5 \), the input signal is smaller than Vdd/2, therefore Ipu(V) is off and Ipd(V) is on, to represent '0'.

The coupling mechanism from DGTD to IBIS can be carried out in a similar way to SPICE, as displayed in Figure 5.10. Within each time step of the above process, a DGTD-IBIS co-simulation looping is performed between the full wave electromagnetic solver and the circuit solver. When the co-simulation goes from one time step \( t^n \) to the next time step \( t^{n+1} \), DGTD sends \( V^n \) and \( V^{n+1} \) to the IBIS circuits, then the simulation of IBIS circuits is performed from \( t^n \) to \( t^{n+1} \). The result of IBIS simulation \( I_{CKT} \) is sampled at \( t^{n+1/2} \) and sent back to DGTD for the EM simulation.
The communication between the DGTD and IBIS solvers will be executed iteratively until a predefined tolerance is satisfied.

### 5.4 EM and Circuit Co-Simulation Scheme

[Diagrams showing field update routines in EM-circuit co-simulation from $n\delta t$ to $(n + 1)\delta t$.]

Combining with the previously mentioned formulations and implementations, the proposed self-consistent DGTD-circuit co-simulation approach can be formally stated as:

1. We start from time $t^n = n\delta t$, with $V^n_{EM} = V^n_{CKT}$.

2. For the pure EM part, DGTD will be executed from $t^n$ to $t^{n+1}$ through (5.15).
3. By setting the iteration number $k = 0$, we make an initial guess of the voltage across the circuit as $V_{\text{CKT}}^{n+1,k} = V_{\text{CKT}}^n + (V_{\text{CKT}}^n - V_{\text{CKT}}^{n-1})$

4. In the SPICE or IBIS circuit solver, the initial conditions at $t^n$ are updated, including all the historical circuit states such as node voltages and branch currents. This is done by reading the simulation results from the previous time step.

5. SPICE/IBIS circuits take a linear driving source defined from $t^n$ to $t^{n+1}$. The source is constructed as $V_{\text{CKT}}^n$ at $t^n$ and $V_{\text{CKT}}^{n+1,k}$ at $t^{n+1}$.

6. With all the initial conditions and voltage source, the circuit solver performs transient simulation from $t^n$ to $t^{n+1}$ by (5.27). $I_{\text{CKT}}^{n+\frac{1}{2},k}$ will be saved and sent to the EM part.

7. In the EM subsystem, the elements that touch the circuit port are solved by DGTD with the current density $J_{\text{CKT}}^{n+\frac{1}{2},k} = I_{\text{CKT}}^{n+\frac{1}{2},k} / w$ through (5.24). After DGTD finishes running, we compute $V_{\text{EM}}^{n+1,k}$ via (5.26).

8. Check whether

$$\frac{|V_{\text{EM}}^{n+1,k} - V_{\text{CKT}}^{n+1,k}|}{|V_{\text{CKT}}^{n+1,k}|} < \epsilon$$

(5.28)

If not, $k = k + 1$, calculate $V_{\text{CKT}}^{n+1,k+1}$ through (5.8) and (5.6), and go to step 5. Otherwise, go to the next steps.

9. The simulation from $t^n$ to $t^{n+1}$ is completed. $V_{\text{CKT}}^{n+1}/V_{\text{EM}}^{n+1}$ will be saved as well as the final circuit states at $t^{n+1}$.

10. The magnetic fields are updated from $H^{n+\frac{1}{2}}$ to $H^{n+\frac{3}{2}}$ by (5.16) and (5.25).
The co-simulation from $t^n$ to $t^{n+1}$ begins. Go to step 1.

Figure 5.11 sketches the co-simulation details from $t^n$ to $t^{n+1}$. Note although we illustrate our method by using only one port, the co-simulation method can be easily extended to multi-port cases as well.

5.5 Numerical Examples

To test the reliability of the developed method, two examples with nonlinear circuit components are presented. The first example is solved by applying DGTD-Ngspice co-simulation, while the second one is simulated with the developed DGTD-IBIS approach. In DGTD, we employ the first order absorbing boundary condition. Moreover, the linear basis functions are used for both the electric and magnetic fields. The two models are also established in CST [79], where the simulation results are used as the references.

5.5.1 A Step Recovery Diode Based Pulse Generator

In this example, we consider the numerical analysis of a pulse generator based on a step-recovery diode (SRD). As shown in Figure 5.12, the pulse generator consists of coplanar waveguide layout (substrate material is FR4) with traces, grounding vias, and

<table>
<thead>
<tr>
<th>$w_1$</th>
<th>$w_2$</th>
<th>$w_3$</th>
<th>$l_1$</th>
<th>$l_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5 mm</td>
<td>1.25 mm</td>
<td>0.20 mm</td>
<td>3.75 mm</td>
<td>0.50 mm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$l_3$</th>
<th>$l_4$</th>
<th>$s$</th>
<th>$h$</th>
<th>$d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.50 mm</td>
<td>0.75 mm</td>
<td>0.50 mm</td>
<td>0.40 mm</td>
<td>0.20 mm</td>
</tr>
</tbody>
</table>
inductor, two capacitors and a SRD. The detailed geometrical parameters are listed in Table. 5.1, while the circuit layout of the pulse generator are depicted in Figure 5.13. Furthermore, the SPICE model of the SRD is detailed in Table 5.2. The capacitor in parallel and the inductor in series with it represent the parasitic elements of the SMD package.

As aforementioned, the EM part will be solved by DGTD while the circuit part are passed into Ngspice through the form of SPICE netlist. The two subsystems are connected through planar circuit ports, as shown in Figure 5.1.

The pulse generator is driven by a sinusoidal voltage source with an amplitude of 2.36 Volts and frequency of 60 MHz. By examining the structure carefully in Figure 5.13, we can get a understanding of how the pulse generator works. At port 1, a low-frequency harmonic signal is excited. The signal passes through a LC low-pass filter (port 3 and port 4) and reaches at the SRD package at port 5. Here, the SRD acts

Figure 5.12: Schematic structure of the SRD pulse generator.
Figure 5.13: EM and circuit co-simulation diagram of the SRD pulse generator.

Table 5.2: SPICE Model Description of the Step-Recovery Diode

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>IS</td>
<td>Saturation current per unit area</td>
<td>0.5 pA</td>
</tr>
<tr>
<td>RS</td>
<td>Ohmic series resistance</td>
<td>0.13 Ω</td>
</tr>
<tr>
<td>N</td>
<td>Emission coefficient</td>
<td>1.3</td>
</tr>
<tr>
<td>VJ</td>
<td>Contact potential at area junction</td>
<td>0.5 V</td>
</tr>
<tr>
<td>M</td>
<td>Grading coefficient at area junction</td>
<td>0.235</td>
</tr>
<tr>
<td>BV</td>
<td>Reverse breakdown voltage</td>
<td>60 V</td>
</tr>
<tr>
<td>IBV</td>
<td>Current at breakdown voltage</td>
<td>10 µA</td>
</tr>
<tr>
<td>TT</td>
<td>Transit time</td>
<td>30 ns</td>
</tr>
<tr>
<td>FC</td>
<td>Coefficient for forward-bias depletion bottom-wall capacitance formula</td>
<td>0.8</td>
</tr>
</tbody>
</table>
Figure 5.14: Result comparison of the voltages at the output side of the SRD pulse generator between DGTD and CST reference.

Figure 5.15: Result comparison of the currents at the input side of the SRD pulse generator between DGTD and CST reference.
as a charge controlled switch for waveform sharpening. During the first half period of the input sinusoidal signal, the SRD is charged by positive voltages and behaves as nearly shorted. While at the second half period, the SRD is being discharged by negative voltages. Once its charges is depleted, the strong non-linearity of the SRD will cause the impedance to change very sharply from nearly zero to an extremely large value. In this way, the signal is blocked by the diode, is filtered by the DC blocking 1.5-pF capacitor at port 6, and produces a sub-nanosecond pulse at port 2. The numerical results in Figures 5.14 and 5.15 confirm the theory, where Figure 5.14 shows the transient voltages at port 2, and Figure 5.15 draws the sampled currents at port 1. Moreover, the numerical results matches the CST results very well.

5.5.2 The Simulation of A Multilayer PCB System

To validate the IBIS circuit simulation and the integration of DGTD and IBIS simulations, we herein present a seven-layer PCB model, as shown in Figure 5.16. The model is export from the PCB studio of CST [79] and the 3-D geometrical details of the model is displayed in Figure 5.17 and Figure 5.18. The lumped elements at the first and seventh layers are modeled as impedance surfaces [47], as depicted in Figure 5.19.

There are five surface mount chips in the problem. One is a 32-bit microprocessor, which is based on the MPC5200 of [90]. The other four are 512 MB DDR SDRAM chips [91]. All of them are provided in the formats of IBIS models. As described in previous sections, they will be solved in a separate circuit solver. Surface circuit ports are used to connect them to the DGTD simulation. Herein, we construct the circuit ports between the PEC pads/traces and the nearest ground plane, as shown
Figure 5.16: A seven-layer PCB model.

Figure 5.17: Geometrical details of the PCB model.
Figure 5.18: Schematic illustration of the seven-layer geometries.
Figure 5.19: Impedance surfaces that represent the R, L, C elements in the top and bottom of the PCB.

Figure 5.20: (a) The microprocessor chip and the corresponding 3-D geometry; (b) The memory chip and corresponding 3-D geometry.
Figure 5.21: Simulation setup of the PCB model. Five rectangular pulse excite the output buffers of the microprocessor chip. The signals go into the PCB and are received at the input buffers of the memory chips.

in Figure 5.20. For simplicity and convenience, five selected pins in each chips are modeled and passed into simulation.

Figure 5.21 presents the simulation settings of the problem. Five identical rectangular pulses are given to drive the IBIS output buffer in the microprocessor. The signals are received at the IBIS input buffers in each of the memory chips. As can be seen, the geometry of the entire model is very complex. To handle the simulation, we employ nonconformal domain decomposition in DGTD. Firstly, each layer of the PCB problem are modeled and meshed independently. Herein, note the meaning of the layer is associated with mesh layers, which is different from the PCB terminology. There are ten mesh layers in total: six substrate mesh layers, two solder mask layers, and two air box layers. Secondly, we conformally partition the mesh in each layer into smaller subdomains [92]. The partitioning is done with respect to the amount of
Figure 5.22: Domain and mesh partitions for DGTD simulation. The layers are meshed nonconformally. In each layer, the meshes are further partitioned into smaller subdomains. Each subdomain is mapped to a MPI process.

float point operations (FLOs) in all the elements, so that the split subdomains can have similar amount of FLOs. The balancing strategy is detailed in [59]. The only difference here is that the FLOs for the circuit simulation also need to be considered for the related elements that touch the circuit ports. Those elements will have higher FLOs than the pure EM elements. The mesh and domain partition results are demonstrated in Figure 5.22.

Finally, we map each subdomain into a MPI process and simulate the problem through MPI parallelization. The simulation is conducted at the Oakley cluster of the Ohio Supercomputer Center [93]. The simulation information are summarized in Table 5.3 and the simulation results are presented from Figure 5.23 to Figure 119.
Table 5.3: Computational Statistics of the Multilayer PCB Simulation.

<table>
<thead>
<tr>
<th>Number of subdomains</th>
<th>DOFs</th>
<th>Local time stepping groups</th>
</tr>
</thead>
<tbody>
<tr>
<td>998</td>
<td>59,646,408</td>
<td>5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation time</th>
<th>Number of time steps</th>
<th>Average cost per time step</th>
</tr>
</thead>
<tbody>
<tr>
<td>35 h 21 min</td>
<td>107,530</td>
<td>1.2 s</td>
</tr>
</tbody>
</table>

5.27. Reasonable agreements can be observed between the DGTD-IBIS co-simulation results and CST reference results.

In addition, in the simulations of both examples, for a relative error tolerance of $\epsilon = 1 \times 10^{-6}$, the proposed self-consistent method is able to converge at each time step within an iteration number $k$ of four. Nevertheless, the simulation, as shown in Table 5.3, is still quite expensive considering the computational resources it consumes. The biggest reason for such inefficiency is the time step. Because we use explicit time marching scheme, the time step is determined by the effective radiiuses of the tetrahedral elements. If a tetrahedron is long and thin, the associated time step can be constrained to be very small. Even if local time stepping approach is used, the efficiency of DGTD, however, can still be deteriorated when the majority of the local time steps are small. Consequently, one remedy for such problem is to employ prism elements, where the total DOFs can be reduced and the time steps can also be increased. An alternative is to apply implicit method for DGTD. In that case, the time step should not be limited by the tetrahedral element shapes, thereby enhancing the computational efficiency.
Figure 5.23: The transient voltage response at pin C20 of the microprocessor chip.

Figure 5.24: The transient voltage response at pin 37 of the first memory chip.
Figure 5.25: The transient voltage response at pin 40 of the second memory chip.

Figure 5.26: The transient voltage response at pin 37 of the third memory chip.
Figure 5.27: The transient voltage response at pin 38 of the fourth memory chip.
Chapter 6: Conclusions

In this dissertation, we have investigated the numerical simulation of radio frequency devices in frequency domain and time domain. The frequency-domain methods and analyses are developed in Chapters 2, 3, and 4, while Chapter 5 studies the time-domain computation.

For time-harmonic electromagnetic applications, an embedded domain decomposition algorithm is proposed to solve a problem with a set of completely nonconformal subdomains: a background that includes the basic shape of the problem and several embedded meshes that contain the geometrical details. Due to the introduction of the embedded meshes, the details of a problem can be decoupled and modeled in different subdomains. The couplings between the subdomains are formulated by analyzing field continuity, material difference, the existence of PEC and port. Direct solver is employed for each of the subdomains while the communications between them are achieved by iteratively imposing coupling sources.

Following the formulation of embedded DDM, we carry out the numerical studies of the method with respect to accuracy, iterative convergence, and h-convergence. Very encouraging numerical properties have been observed. Moreover, the implementation details of the integration on the subdomain interface, as well as the transmission condition between the touched embedded meshes, have been examined through two
experiments. Furthermore, we apply embedded DDM to solve three types of practical problems: EM environments, antenna simulation, and IC analyses. As clearly shown in those examples, the biggest benefit of embedded DDM is its flexibility in utilizing completely nonconformal meshes, so that the model and mesh preparation stages for numerical simulation can be significantly sped up. The method should be suitable for design and optimization problems, especially when the components in the problem are required to be modified frequently.

For mixed EM and circuit scenarios, initially, a problem is decomposed into two subsystems. The EM subsystem is solved with DGTD simulation by acquiring the currents from the circuit subsystem. The simulation of the circuit subsystem is conducted with the voltages obtained in EM. We have argued that, in order to link the two subsystems rigorously, a self-consistent condition should be ensured throughout co-simulation. Under such conclusion, we have built an iterative methodology by using planar circuit ports with respect to voltage and current continuities. The application of the method is examined with a pulse generator and a multilayer PCB system. The simulation results agree well with the references, and the capability and accuracy of the developed method are demonstrated in addressing mixed EM and circuit problems.

Regarding the directions of future research, we mention a few here. Firstly, a large number of real-life EM devices include duplicated or symmetric components, such as metamaterials and antenna arrays. Embedded meshing technique is well suited for exploiting the repetition nature of such structures, so that tremendous computational efforts may be saved. Moreover, embedded DDM with subdomains adopting different types of meshes (tetrahedron, prism, brick) is also an interesting topic. Because in
this way, appropriate meshing shapes can be chosen for different components in a problem. Furthermore, the time-domain counterpart of embedded DDM as well as its marriage with the approach in Chapter 5 will certainly worth investigation.
Bibliography


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