Hybrid Models for Parasitic Capacitances in Advanced VLSI Circuits

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Hybrid Models for Parasitic Capacitances in Advanced VLSI Circuits

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Chapter 1

INTRODUCTION

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1.1 Extraction problems in verification of the behavior of IC's

Current trends toward increased packaging density of integrated circuit have resulted in very small device dimensions and proximity. To achieve high packaging density modern technology must offer multilevel interconnects. This is due to the fact that the topology of complex wiring cannot be put into a single level of metalization without line crossings. Thus, advanced technologies provide increasing number of interconnect layers, from straps between the polysilicon interconnect layers and the so-called “diffusion” paths in the silicon substrate, to metal-one, metal-two and more metal layers (four, five already and seven in the future).

The reduction of the physical dimensions of devices can be obtained by scaling. Linear scaling in all three dimensions implies that the width and the height of conductors shrink at the same rate as the dielectric layer thickness, resulting in an unwanted excess increase of the wire resistance. Hence, lateral scaling is applied to the metal interconnects, leaving the vertical dimension intact to assure a sufficiently
low current density. As a result, the ratio of interwire capacitance to ground capacitance increases, and makes the former play a larger role. Therefore, the two-dimensional fringing fields and the capacitances between neighboring lines must be taken into account. Moreover, increasing the number of dielectric layers will make the capacitances between interconnects in different layers larger. With constant increase of the complexity of IC's the length of the wires running through the IC becomes relatively long. The parasitic effects on wires, such as non-negligible resistance, have been gaining increasing importance. We can conclude that with reducing dimensions and increasing packaging density, the \textit{global parasitic effects}, such as wire resistance and interwire capacitances, are playing a very important role in the circuit performance and must be taken into account in the design process. These effects are particularly critical for high frequency circuits in the Giga-Hertz range. Here parasitic effects can result in bit errors for digital circuits and considerable changes in the signal for analog circuits.

Our main focus in this dissertation, will be on the self and coupling capacitances for IC interconnect since they are essential for determining final circuit performance and reliability. Especially, precise estimation of \textit{parasitic capacitances} is one of the most important aspects in designing high performance VLSI circuits. The knowledge of capacitances can be used to predict circuit switching speed. But parasitic capacitances cause undesirable circuit behavior. Thus there is a large need for a good estimation of values for the parasitic capacitances.

Designers of modern IC's rely heavily on the \textit{layout-to-circuit extraction} systems, which for a given layout design of the circuit compute an equivalent model in the form of an electrical circuit. The subsequent simulation of the equivalent electrical model allows to verify the correct behavior of IC before costly fabrication. The process in which the capacitances are determined from the layout of the circuit we call \textit{capacitance extraction}.

Until now, the \textit{boundary element method} (BEM) [Ruehli 73], [Brebbia 78], [Dewilde 90], [Meijs 92] and the \textit{finite element method} (FEM) [Norrie 73], [Silvester 83], [Livesley 83] are the most popular techniques used for accurate capacitance modeling.

The BEM is based on the assumption that the structure of IC's may be well approximated by a uniform stratification of dielectric layers bordered at the bottom by ideal ground plane, whose potential is zero. The conductors running through such a dielectric structure are assumed to be perfectly conducting and each of them forms an equipotential.

For calculation of multiconductor capacitances, the BEM allows one to express the electrostatic potential in terms of \textit{prime integrals} known as \textit{Green's functions}. However, the BEM can only be used when the Green's function is readily given, i.e. when the stratification of the dielectric layers is perfect, as is illustrated in Figure 1.1(a). If the dielectric structure of the integrated circuit becomes irregular, e.g. disturbances in planarization of dielectric interfaces or regions where the
1.1 Extraction problems in verification of the behavior of IC's

dielectric permittivity varies irregularly, the Green’s function method loses much of its usefulness. Then one must resort to the FEM.

\[ k_1 \quad k_2 \]

\[
\text{ground plane} \quad \text{ground plane}
\]

(a) (b)

Figure 1.1. (a) Example of a stratification for which the BEM can be used. (b) Example of a stratification for which the HEM can be used.

The FEM solves the differential equations, which govern the electrical field in large scale integrated circuits, in a closed, relatively small domain directly and locally. But the FEM results in a very large, although sparse, system of linear equations when it models the entire layout of IC. The other disadvantage of the FEM, in comparison with the BEM, is that it cannot handle well the effects of an electrical field which extends to infinity.

Taking into account all the advantages and disadvantages of the two techniques, it seems to be very attractive to combine these two methods maintaining the best features of the methods themselves.

In this dissertation we propose a new version of a hybrid element method (HEM) for the modeling of capacitive interconnects which is capable of dealing efficiently with disturbances and/or irregularities in a dielectric stratification, as is illustrated in Figure 1.1(b). The key concept of our method is to combine the BEM and the FEM in one capacitance extraction system, so that the BEM is used in the regular regions of the layout of IC, while the FEM is used in the bounded, localized regions that exhibit irregularities. HEM profits from the advantages of both the BEM and the FEM and avoids their disadvantages.

The derivation of the capacitance models for either the BEM [Ruehli 73], [Balaban 73], [Ruehli 75] or the FEM [Cottrell 85], [Straker 86] are well established. Thus, the main modeling problem to be considered is how to connect the two models obtained by the BEM and the FEM. There are many ways to tackle this problem.

The idea of coupling the BEM with the FEM is not new. Some proposals for the BEM/FEM modeling can be found in the literature, e.g. [Pridmore 81], [Gupta 87], [Ren 88], [Pichon 89], [Costabel 90], [Everstine 90], [Jeans 90], [Hirayama 92],
[Wu 92], [Jeans 93], [Chen 94], [Gong 94]. However, they are dedicated to problems in e.g. seismology, acoustics and elasticity, so they are used in different contexts and with different requirements. The hybrid BEM/FEM methods for electrostatics focus on solving particular field problems and do not give a good physical circuit model, which is desired for extraction purposes. As well as this, the previously known methods were iterative, which implies that it is impossible to construct the model.

Our proposal for the electrical model of the interface between regions modeled by the BEM and the FEM is a generalized ideal transformer [Belevitch 68]. A complete circuit model then consists of a lossless system of capacitances coupled by ideal transformers. Subsequent elimination of the transformers yields a purely capacitive model. From this model one can easily derive all the coupling capacitances as desired.

Our hybrid element method has been validated and tested for basic benchmarks with layered media in two and three dimensions. Theoretically we found good convergence properties of the hybrid method. These have been confirmed by practical results.

Comparison of results obtained by the HEM and other methods will show the usefulness and superiority of the hybrid method.

The sequel of this introduction is devoted to:

1. mathematical background from the theory of electrostatics;
2. overview of methods used for capacitance extraction.

### 1.2 Mathematical description of the electrostatic field

To describe both the spatial and the temporal behavior of the electric field within a complex interconnection environment, it would be necessary to obtain the solution of the complete set of Maxwell’s equations. But assuming that the frequencies at which IC’s are working are low enough, we can neglect the temporal derivative of the magnetic field. Thus the complete set of Maxwell’s equations can be reduced to the electrostatic case governed by Laplace’s equation while still accurately describing the field distribution.

The boundary conditions, which complete the necessary set of equations are of the Dirichlet or Neumann type or mixed. When the boundary field is known or specified we have a Dirichlet type, when the normal derivative is given the type is Neumann.

We use the following notation:
1.2 Mathematical description of the electrostatic field

\( \Omega \) - an open volume;
\( S \) - its enclosing boundary surface (sufficiently smooth);
\( p \) - a point with coordinates \((x_p, y_p, z_p)\) in \( \Omega \cup S \);
\( n \) - the outward normal to a surface \( S \);
\( dp \) - depending on the context an element on the surface area or an element of the volume in which point \( p \) is located;
\( \vec{D}(p) \) - the electric flux density at a point \( p \);
\( \vec{E}(p) \) - the local electric field in a point \( p \);
\( k(p) \) - the permittivity of the medium at a point \( p \), given as the product of the relative permittivity of the medium \( \varepsilon_r \) and the absolute permittivity of free space vacuum \( \varepsilon_0 \);
\( \rho(p) \) - the charge density in the volume \( \Omega \);
\( \nabla \) - the gradient operator \([\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}]^T\).

For the sake of clarity and to obtain less cluttered formulas, we use notation \( n \) instead of \( \vec{n} \), the same holds for certain other specified vectors such as \( \vec{p} \), \( q \) etc.

The flux density and the local electric field are related by:

\[ \vec{D}(p) = k(p)\vec{E}(p). \tag{1.1} \]

For a continuous charge density \( \rho(p) \) and any volume \( \Omega \) with smooth surface \( S \), Gauss’s dielectric flux theorem [Jackson 75], [Weber 54] gives the following integral form:

\[ \int_{p \in S} (\vec{D}(p) \cdot n) \, dp = \int_{p \in \Omega} \rho(p) \, dp. \tag{1.2} \]

Since

\[ \int_{p \in S} (\vec{D}(p) \cdot n) \, dp = \int_{p \in \Omega} \nabla \cdot \vec{D}(p) \, dp, \tag{1.3} \]

and \( \Omega \) is otherwise arbitrary, this is equivalent to the differential form:

\[ \nabla \cdot \vec{D}(p) = \rho(p). \tag{1.4} \]

Moreover, because of the frequency assumption, the electric field is curl-free. This allows us to derive the electric field from a scalar potential \( \Phi \) by a gradient operation [Duffin 80], [Jackson 75]. The expression for the local electric field \( \vec{E} \) becomes:

\[ \vec{E}(p) = -\nabla \Phi(p). \tag{1.5} \]

Combining Equations (1.1), (1.4) and (1.5) we arrive at the following partial differential equation:

\[ \nabla \cdot [k(p)\nabla \Phi(p)] = -\rho(p), \tag{1.6} \]

which evaluates to the formula:

\[ \nabla \cdot [k(p)\nabla \Phi(p)] + k(p)\nabla ^2 \Phi(p) = -\rho(p), \tag{1.7} \]
known as Poisson’s equation.

For a homogeneous medium, when \( k(p) = k = \text{constant} \), Equation (1.7) reduces to:

\[
\nabla^2 \Phi(p) = -\frac{\rho(p)}{k}. \tag{1.8}
\]

Moreover, if there are no volume charges present in the space under consideration we have a further reduction to the so-called Laplace’s equation:

\[
\nabla^2 \Phi(p) = 0. \tag{1.9}
\]

### 1.3 Integral equations

Let us now consider a system of conducting bodies floating in a homogeneous dielectric medium with constant permittivity \( k \) and of infinite dimensions. The electric field surrounding the ideal conductors is governed by Laplace’s equation. Its formal solution [Weber 54] can be written as:

\[
\Phi(p) = \int_{q \in \Omega} \frac{1}{4\pi k} \frac{1}{|p - q|} \sigma(q) \, dq. \tag{1.10}
\]

where \(|p - q|\) denotes the Euclidean distance between points \( p \) and \( q \), \( \sigma(q) \) is the charge density at the point \( q \). The factor:

\[
\frac{1}{4\pi k} \frac{1}{|p - q|} \tag{1.11}
\]

is called the Green’s function \( G(p, q) \) for a uniform dielectric medium of infinite dimensions, or shortly; the free space Green’s function, with the permittivity \( k \). The Green’s function can be interpreted as the potential induced at point \( p \) due to a unit point charge at \( q \). The point \( p \) is called the observation point and \( q \) is called the source point.

Now Equation (1.10) can be written as:

\[
\Phi(p) = \int_{q \in S} G(p, q) \sigma(q) \, dq. \tag{1.12}
\]

Consider a system of (charged) conductors as depicted in Figure 1.2. A perfectly conducting ground plane is shown and three conductors floating in a medium consisting of dielectric layers with permittivity \( k_i \) of each layer. The charges on the conductors are represented by a charge density \( \sigma(q) \). We shall show in the next sections that for such a dielectric stratification the Green’s function can be found, and the formal solution to the field problem is given by Equation (1.12). If Equation (1.12) is specialized to a point \( p \) on the surface of the \( i^{th} \) conductor with the
1.4 Overview of methods used for capacitance extraction

1.4 Overview of methods used for capacitance extraction

Several methods have been used to obtain capacitances for signal lines. These include:

- exact closed-form solution;
- approximate formulas, e.g. area-perimeter formulas;
- detailed numerical solution.

Closed-form exact solutions can be obtained in 2D and 3D for symmetrical geometries by using separation of variables or by conformal mapping [Chang 76]. The exact solutions are elegant but they are limited by the geometries that they can handle. Certainly they are unable of handling geometries of advanced integrated circuits.

Approximate formulas are usually based on analogy between the actual geometry and an idealized geometry for which we can find an exact solution [Yuan 82], [Sakurai 83], [Uyemura 92]. The other way of getting simple formulas is to fit
curves to capacitance values calculated numerically. The approximate formulas should be verified by hardware measurements and/or detailed numerical calculation in order to produce sufficiently accurate values for IC's.

**Numerical methods** for calculating capacitances are convenient and fast alternatives when physical measurements or closed-form solutions are difficult to obtain.

### 1.4.1 Numerical methods for capacitance extraction

We can distinguish two basic groups of methods which exist for the numerical calculation of capacitances:

- methods that solve for the potential through space, e.g. the finite difference method (FDM) [Dierking 82], [Taylor 85], [Seidl 88], [Guerrieri 88] and the finite element method (FEM) [Cottrell 85], [Straker 86] which are based on the differential form of the electrostatic equations;

- methods that solve for the charge density, i.e. the boundary element method (BEM) often called the integral equation method since it is based on the integral form of the electrostatic equation.

Each of these methods has advantages and disadvantages, and with respect to many properties they are complementary.

### 1.4.2 The finite element method and the finite difference method

The main disadvantage of the FEM and the FDM is that they must fill all the space, in which we solve the differential equations, with a finite element mesh. Therefore, the FEM may require an extremely large number of unknowns in order to obtain a good accuracy. Its complexity gets out of hand when the size of the region gets larger. Moreover, the potential field must be numerically differentiable to obtain the capacitances. Due to numerical differentiation the method is prone to errors induced by inadequate discretization, including the problem of representing the boundary at infinity. The method is capable of accurate modeling of regions with irregularly varying material characteristics, but can only handle bounded regions. Hence, the applicability of the FEM for global extraction is limited to small, well described regions. It is incapable of handling the far field without major complications. We must always remember that the artificial boundary of the modeled region should be separated from the conductors by a distance that is large compared to the characteristic dimensions of the conductor cross-section.

Advantages of the FEM are:

- the matrix of coefficients of the linear system is extremely sparse;
- the non-zero coefficients in the matrix are easy to calculate;
1.4 Overview of methods used for capacitance extraction

- the matrix of coefficients is symmetric.

Additionally, the FEM can handle complex geometries in a natural and straightforward manner, since in 2D it uses triangular finite elements and in 3D tetrahedral finite elements.

1.4.3 The boundary element method

A method which is well-suited for 3D-modeling and far field effects makes use of a parameterized prime integral of the partial differential equation, the Green's function $G(p, q)$. In capacitance modeling problems, it allows to express the field as a function of the charges on the boundary of conductors. In the boundary element method the unknown is the charge density. We assume that the conductors are perfect. This means that the charge is concentrated only on the surface of conductors. Therefore, we don’t need to discretize the entire space, but only the surfaces on which charge is present. In order to solve the 3D problem we need to discretize a finite 2D surface of conductors, similarly for 2D problem we need to discretize a finite contour consisting of 1D intervals. The number of unknowns is thus smaller than that used by the FEM. This results in a much lower computational complexity for the BEM. Moreover, no numerical differentiation is required in order to obtain the capacitances.

The disadvantage of the BEM is that:

- the matrix of coefficients for the linear system is completely full;
- the evaluation of the entries in the coefficients matrix, i.e. the integration of the Green's function is costly, especially for more complex media such as stratified structures;
- special care is required with the integration over singularities.

The BEM handles correctly the effects of the infinite field by using the proper Green’s function. In the case of the free field in vacuum with no boundary, the Green’s function is given by expression (1.11) with the relative permittivity $k_r = 1$,

$$G(p, q) = \frac{1}{4\pi k_0} \frac{1}{|p - q|}$$

(1.14)

where $p$ is the observation point and $q$ is the source point. In the case of an infinite layered medium, the Green’s function can still be determined, by using Bessel functions [Benedek 76], [Dewilde 90], but its evaluation becomes harder and consumes more time.

If the medium is irregular, e.g. the stratification is imperfect, or the boundary conditions are complex, then the Green’s function method is not attractive anymore.
In this case it is still possible to modify the BEM so that it can handle more complex geometries quite typical for integrated circuits. Examples of such methods are presented by [Ruehli 73], [Patel 71]. Most of them are based on the hybrid boundary element method which uses the free space Green’s function and explicitly treats all the bound charges at the dielectric interfaces. This approach is more flexible in treating the complex dielectric structures but results in a high cost of solving for the bound charge at any infinite dielectric interface.

1.4.4 The hybrid integral methods

The other approach uses the multilayer Green’s function to take into account the effect of the infinite planar dielectric interfaces and an explicit treatment of the bound charge at the finite and irregular dielectric interfaces [Janak 89]. But even so, this hybrid integral method is still limited by allowed geometries. Usually an additional dielectric structure can be created by using finite dielectric bars (rectangular parallelepipeds) having an arbitrary dielectric permittivity. The permittivity cannot vary inside the dielectric bar. Moreover, two dielectric bars cannot partially overlap. Either they are totally disjoint, or one is entirely inside the other.

An hybrid integral method allows to express the electrostatic potential at any point in 3D space as the function of the free and bound charges. The imposed boundary conditions concern both the free and bound charges, and are as follows:

- at dielectric interfaces the normal component of the displacement field must be continuous across the interface (one equation in one unknown — the bound charge);
- the surface of the conductors is equipotential (one equation in one unknown — free charge).

Once the boundary conditions have been imposed, we can solve the set of algebraic equations obtained by using the Galerkin method for the free and bound charges and this yields the capacitance matrix [Ruehli 73], [Ruehli 79].

The hybrid integral method has many advantages but still is not flexible enough to handle irregular dielectric regions in which the permittivity varies.

1.4.5 The BEM and the FEM coupled

An alternative method is to combine the BEM and the FEM for capacitance modeling. But again the coupling can be done in many ways.

First, let us discuss the method presented in [Pridmore 81] and [Gupta 87], applied to electromagnetic problems in which the disturbance (irregularity) of the regular stratification is giving rise to a scattered field added to the background field from the regular, perfect (undisturbed) situation.
1.4 Overview of methods used for capacitance extraction

The hybrid method presented in these papers can be adapted to our modeling problem. The FEM is used only to compute the perturbation of the field due to irregularities in the medium, rather than the field itself. Below, we give a brief description of the method.

Let \( \Phi_b \) be the (primary) "background" potential field which would be present if the layered medium were perfectly stratified. The total field in any point of the domain is:

\[
\Phi = \Phi_b + \Phi_s
\]

(1.15)

where \( \Phi_s \) is the (secondary) "scattered" potential field.

Similarly we express the permittivity as:

\[
k = k_b + k_s
\]

(1.16)

\( k_b \) being the permittivity of the stratified dielectric layers and \( k_s \) its disturbance, which is non-zero only in a very small inhomogeneous region.

The field equations are:

1. for the 'background' field,

\[
\nabla[k_b \nabla \Phi_b] = -\rho
\]

(1.17)

2. for the overall field,

\[
\nabla[k \nabla \Phi] = -\rho
\]

(1.18)

Subtracting (1.17) and (1.18) we obtain:

\[
\nabla[k \nabla \Phi_s] = -\nabla[k_s \nabla \Phi_b]
\]

(1.19)

We assume that the background field \( \Phi_b \) is known. The scattered field \( \Phi_s \) can then be obtained by solving (1.19) using the FEM. In order to formulate the finite element equations, the relevant energy functional must be derived for (1.19) which takes into account the necessary boundary conditions. The energy functional is the volume integral over the domain being modeled of the square of the gradient of the potential. In this case, the domain to be discretized by the finite element mesh consists of the inhomogeneous region plus a boundary layer of one element thick.

We must be very careful to extend the scattered region so that \( k_s = 0 \) in the outermost finite elements (one layer). Using tetrahedral finite elements and linear shape functions, we approximate the scattered field in the \( e^{th} \) element as:

\[
\Phi_s^e(p) = \sum_{i=1}^{4} N_i(p) \phi_{si}
\]

(1.20)
where the \( N_i(p) \) are linear shape functions and the \( \phi_{si} \) are the unknown nodal field values. Moreover, let us split the vector \( \phi_s \) of node scattered potentials into a vector \( \phi_s^i \) of internal node values and a vector \( \phi_s^b \) of boundary node values.

Minimizing the energy functional we obtain:

\[
\begin{bmatrix}
K_{ii} & K_{ib} \\
K_{bi} & K_{bb}
\end{bmatrix}
\begin{bmatrix}
\phi_s^i \\
\phi_s^b
\end{bmatrix}
= -
\begin{bmatrix}
S_i \\
S_b
\end{bmatrix}
\]  

(1.21)

where \( K \) is the stiffness matrix and \( S_i \) and \( S_b \) are the source vectors, both \( K \) and \( S \) are computable from the minimization procedure (see for added information, Chapter 3) and the background field.

The first of the equations in (1.21) yields:

\[
K_{ii}\phi_s^i + K_{ib}\phi_s^b = -S_i
\]

(1.22)

or

\[
\phi_s^i = -K_{ii}^{-1}(K_{ib}\phi_s^b + S_i)
\]

(1.23)

It is now necessary to connect \( \phi_s^b \) with the outside field. This can be achieved by using the Green’s function approach. We rewrite (1.19) as:

\[
\nabla[k_s \nabla \Phi_s] = -\nabla[k_s \nabla (\Phi_b + \Phi_s)]
\]

(1.24)

Using Green’s theorem we can write:

\[
\Phi_s(p) = -\int_{q \in \Omega} G(p,q) \nabla_q [k_s \nabla_q (\Phi_b(q) + \Phi_s(q))] \, dq
\]

(1.25)

since the integral over the boundary surface \( \int_{q \in S} G(p,q) k_s \frac{\partial (\Phi_b(q) + \Phi_s(q))}{\partial n_q} \, dq \) vanishes for \( k_s = 0 \) on the boundary. Now, using the same finite element grid which gives rise to the finite element equation (1.21) we can discretize (1.25) yielding:

\[
\phi_s^b = G\phi_s^i + S_p
\]

(1.26)

with \( G \) and \( S_p \) derived from an optimization procedure. It is easy to notice that only the internal fields appear in the integrand since \( k_s \) is zero in the boundary layer.

Substituting (1.26) into (1.23) we obtain:

\[
\phi_s^i = - (K_{ii} + K_{ib}G)^{-1}(S_i + K_{ib}S_p)
\]

(1.27)

Equations (1.23) and (1.27) give the solution to the specific field problem but the derivation of the relevant circuit model is not straightforward. For model construction purposes the expressions for \( \phi_s^b \) and \( \phi_s^i \) have to be introduced in the overall external field, the contribution of the charges on the conductors in (1.26) and (1.27) must be made explicit and the overall functional relation determined. We conclude
that using the scattered field approach is not too attractive due to difficulties associated with the model derivation, which is our ultimate goal.

The other way to combine the BEM and the FEM is direct. In direct hybrid methods we match fields at the boundary between regions in which the BEM and the FEM are used. There are many papers written about the combination of the two techniques applied in different areas of science, see for example [Ren 88], [Pichon 89], [Costabel 90], [Everstine 90], [Jeans 90], [Hirayama 92], [Wu 92], [Jeans 93], [Chen 94], [Gong 94]. In general they are using the principles of the BEM and the FEM to describe the potential field in the regions where the methods are applied assuming that the potential $\Phi$ and its normal derivative $\frac{\partial \Phi}{\partial n}$ are continuous across the boundary.

We show an overview of the available methods for the capacitance modeling and dependence between them in Figure 1.3.

Our approach, which we present in this dissertation, belongs to the direct hybrid BEM/FEM methods. But, in comparison with the known direct methods, in our method we satisfy the continuity conditions between the regions modeled by the BEM and the FEM in an average sense by imposing certain potential and charge distributions, see [Nowacka 96a], [Nowacka 96b], [Dewilde 96]. The circuit interpretation of the potential and charge distribution is that of a generalized transformer. We have studied the new hybrid model of the interface and are able to show that it is a correct model in the sense that the resulting field converges to the true field when the size ($h$) of the mesh goes to zero. The classical Galerkin convergence proof is not directly applicable here because of the discontinuity of the field at the interface. This produces an essential singularity in the gradient of the field which turns out to contribute a negligible part to the total energy, namely a part that goes to zero as $O(h^2)$ ($h$ the size of the mesh) when the mesh refines. For more details see [Nowacka 96b], and also Chapter 5 in this thesis. The BEM and the FEM, due to the first order discretization and the minimum energy principle, converge linearly with the size ($h$) of the mesh when they are applicable. Because of this fact, the solution can be obtained by minimizing the energies of the individual components of the field, assuming the transformer equations to be in force at the interface.

We will show that, indeed, attractive models can be derived for the hybrid BEM–FEM method. They retain the physical properties of the original, i.e. they are purely capacitive, symmetrical and passive. The disturbance introduced by the interface between the regions converges to zero one order of magnitude faster than the BEM and the FEM themselves. Moreover, we will show that the model can be easily integrated in a layout-to-circuit extraction system due to its local structure. We will discuss the implementation of the hybrid element method for capacitance modeling in the extraction system, putting special emphasis on the integration techniques and 3D mesh generation. We will present the results of the prototype program which uses our hybrid technique. Practical results obtained by using the HEM
Capacitance modeling

- exact closed-form solution
- approximate formulas
- numerical solution

  - FEM
  - BEM
  - coupled BEM/FEM

    - integral methods
    - hybrid integral methods

      - 'scattered' field approach
      - direct methods

Figure 1.3. The review of the methods.
1.5 Overview of the thesis

will show good convergence properties of the new method.

1.5 Overview of the thesis

In Chapter 2, we discuss the mathematics and the theoretical background of the BEM. We show how the BEM can be used to accurately compute the interconnect capacitances. We start off with the boundary integral formulation, which later on is discretized. We discuss different manners of discretization and present one kind of discretization, the most suitable for the hybrid modeling. For chosen discretization we develop an equivalent model in the form of an electrical circuit which consists of multiconductor capacitances. The BEM uses the Green's function which must be specialized to the geometric configuration of the dielectric medium. We show how the Green's function can be evaluated by using Bessel functions. We also discuss how the integral of the Green's function and the integral of its normal derivative can be practically evaluated.

In Chapter 3, we discuss applicability of the FEM to the capacitance modeling problem. We give the theoretical and mathematical background of the method. We show how the equivalent capacitive model for 3D finite element can be constructed. We also explain how to assemble the models of elements into a global capacitive model.

In Chapter 4, we introduce the new HEM which couples the BEM and the FEM for capacitance modeling. We give detailed discussion on model construction by using the HEM. We show how the capacitive models obtained by the BEM and the FEM can be combined by ideal generalized transformers. In addition we explain how the concept of the ideal transformer can be applied to the boundary interface between the regions in which the BEM and the FEM are used. The derivation of the multiconductor capacitances by elimination of the transformers follows.

In Chapter 5, we discuss the convergence of the hybrid method. First, we consider different measures, error estimates and the nature of their convergence. We show that the FEM and the BEM themselves converge linearly in the energy norm. Afterwards, we show that the energy associated with the discontinuity of the field at the boundary interface contributes a negligible part to the total energy, namely a part that goes to zero quadratically as the mesh gets finer.

Chapter 6 contains practical results of experiments done by using the hybrid modeling. In this chapter we consider many benchmarks in 2D and 3D space. We make an extensive comparison of the results obtained by the HEM with results coming from the BEM and the FEM themselves. These experiments confirm the good convergence properties of the hybrid method.

In Chapter 7, we consider possible extensions and applications of the HEM to other problems than capacitance extraction.
In Chapter 8, we study how the hybrid method can be incorporated in the layout-to-circuit extraction system. First, we present the prototype implementation of the HEM capable of handling simple geometries. Second, we discuss how the method can be integrated in a modern extraction system. We focus mainly on 3D mesh generation and the scanline technique for the hybrid modeling.
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Chapter 2

THE BOUNDARY ELEMENT METHOD

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2.1 Introduction

The modeling of interwire capacitances brings the "exterior problem" of the Laplace equation into play. In the exterior problem the electric field is not confined to a small, finite domain in the immediate neighborhood of the conductors but it extends to infinity.

One of the most popular methods dealing with the exterior problem is the boundary element method. The method uses the Green's function for conductors in an infinite, uniform or layered dielectric medium [Ruehli 73], [Ruehli 75], [Balaban 73], [Patel 71]. This approach maps the exterior problem into a finite boundary problem on the surface of the conductors using Green's theorem. Since the resulting integral equation is defined only on the finite boundaries of the exterior problem, namely the surface of conductors, only this surface must be discretized. Using the weighted residual method (WRM) on the boundary integral equation, a set of linear equations is obtained from which the capacitances can be deduced.

There are different kinds of the boundary element method depending on the type of the weighted residual procedure which is used. In the literature we can find the following methods which are commonly used in modeling problems: the method of subareas [Ruehli 73], the Galerkin method [Silvester 83], and the point fitting method [Balaban 73].

The boundary element method has proven itself to be a powerful tool in the modeling of 3D multiconductor structures. The method can handle complex geometries of conductors in stratified media. It can not only handle parallel conductors, but also crossing lines, contacts and their combinations. Since the method can be applied to any assembly of elements on conductors, it is well suited for extraction purposes.

A practical example of a successful implementation of the BEM in an extraction system is the (commercially available) extraction package Space (=Submicron Parasitic Artwork to Circuit Extractor) [Meijs 92], [Meijs 94].
2.1 Introduction

2.1.1 Assumptions on the approximation of the dielectric structure of IC's

Before introducing the boundary element technique we make the following assumptions:

1. We consider the electrostatic case only. This assumption is a valid approximation of the physical situation in most of the cases, and only becomes invalid for signals well into the Giga-Hertz spectrum. For GHz frequencies, the decrease of the size of the features of VLSI circuits has lead to geometries in which most of the coupled elements are in very close proximity of each other, to within one wavelength. The assumption about frequencies allows us to reduce Maxwell's equations to electrostatic equations such as Laplace's equation.

2. A reasonable approximation of the structure in which interconnects are located is that of a uniform stratification of dielectric layers, bordered at the bottom by an ideal conductor plane whose potential we assume to be zero [Ruehli 73]. Usually the dielectric structure is considered as a sandwich of essentially silicon dioxide (SiO$_2$), and silicon nitride (Si$_3$N$_4$) delimited at the bottom side by a conducting layer of higher doped silicon and at the top side by a coating and by air. This assumption corresponds to the case in which the surface of the IC is perfectly planarized between each dielectric layer.

3. The conductors running through the sandwich of dielectric layers are supposed to be perfect, i.e. to have an infinite conductance. Each of the conductors forms an equipotential. The field inside the conductors is negligible, and hence the charge essentially accumulates on the surface of the conductors.

4. We assume that the highly doped silicon substrate forms a ground plane. This means that the silicon substrate acts as a highly conducting electrical plate. However, only at very high frequencies the entire substrate plays a role [Hasegawa 71]. The assumption, that the ground plane is a perfectly conducting plane no longer holds, and we need to take into account the dielectric properties of the ground plane.
2.1.2 Short description of the boundary element method for capacitance extraction

Consider a domain $\Omega$ with the dielectric permittivity $k$ and the boundary $S$.

Let:

- $\Phi(p)$ - be the potential at a point $p$;
- $k(p)$ - the permittivity of the medium at a point $p$, given as the product of the relative permittivity of the medium $k_r$ and the absolute permittivity of free space vacuum $k_0$;
- $S(q)$ - the charged surface on which a point $q$ is located;
- $\frac{\partial}{\partial n_q}$ - the derivative along the outward normal $n_q$ to the boundary surface $S(q)$;
- $\sigma(q)$ - the charge density along $S(q)$ given by $\sigma(q) = k(q) \frac{\partial \Phi(q)}{\partial n_q}$;
- $G(p, q)$ - the Green’s function.

The BEM, employed to solve the modeling problem, can be described briefly as follows:

1. Green’s theorem [Hoop 68], [Brebbia 78] for a point $p$ on the surface $S$ yields:

$$\frac{1}{2} \Phi(p) + \int_{q \in S} \Phi(q) k(q) \frac{\partial G(p, q)}{\partial n_q} dq = \int_{q \in S} G(p, q) \sigma(q) dq; \quad (2.1)$$

2. The discretization of the conductor charge as a piecewise constant distribution over a set of the triangular finite elements provides:

$$\sigma(q) \approx \bar{\sigma}(q) = \sum_{i=1}^{N} \sigma_i f_i(q), \quad (2.2)$$

where $f_i(q)$ is the constant shape function assigned to the boundary element $S_i$, and such that $\int_{S_i} f_i(q) dq = 1$;

3. The Galerkin method [Mikhlin 67] applied to the discretized Equation (2.1) gives:

$$G^{-1}[\frac{1}{2} I + G^{(n)}] \Phi = \sigma, \quad (2.3)$$

with:

- $\Phi = [\Phi_1 \Phi_2 ... \Phi_N]^T$ and $\sigma = [\sigma_1 \sigma_2 ... \sigma_N]^T$ the element potentials and element charges, respectively;
- $G^{(n)}$ the matrix with entries:

$$G^{(n)}_{ij} = \int_{p \in S_j} \int_{q \in S_i} k(q) \frac{\partial G(p, q)}{\partial n_q} f_i(p) dq dp; \quad (2.4)$$
2.2 Boundary integral formulation

- $G$ the matrix with entries:
  \[ G_{ij} = \int_{p \in S_i} \int_{q \in S_j} G(p, q) f_j(q) f_i(p) \, dq \, dp; \]  
  (2.5)
- $I$ the identity matrix;

4. The symmetrization of the capacitance matrix $C_c = G^{-1}\left[\frac{1}{2} I + G^{(n)}\right]$ by substitution (this substitution will be justified later):
  \[ C = \frac{1}{2} [C_c + C_c^T] \]  
  (2.6)
provides the matrix equation:
  \[ C\Phi = \sigma; \]  
  (2.7)

5. The calculation of the conductor capacitances is done by use of an incidence matrix $A$ such that $A_{ij}$ is 1 if element $i$ lies on conductor $j$, and zero otherwise. Let $V = [V_1 V_2 ... V_M]^T$ be the vector of conductor potentials and $Q = [Q_1 Q_2 ... Q_M]^T$ the vector of charges on conductors. The following derivation is then valid:
  \[ Q = A^T \sigma = A^T C\Phi = A^T C A V = C_s V, \]  
  (2.8)
where $C_s = A^T C A$ is the so-called short-circuit capacitance matrix and is the matrix to be calculated.

Each of the above steps will be treated in greater detail in the following sections.

2.2 Boundary integral formulation

To solve the “exterior problem” for the Laplace equation and relate the solution to the boundaries, the surface of conductors, we use Green’s theorem. We develop this boundary formulation step by step. We start off with a so-called first Green’s theorem for a closed region. Then we formulate second and third Green’s theorem for the closed region.

To derive the third Green’s theorem for an open infinite region we use an equivalent formulation for a closed region. We introduce an artificial boundary which we move in the limit to infinity obtaining the boundary formulation for an open infinite domain. Finally, we derive the boundary integral equation for the open region outside the equipotential surface.
2.2.1 Boundary integral formulation for a closed domain

Let $\Omega$ be a dielectric region, with constant dielectric permittivity $k$, surrounded by a sufficiently smooth boundary $S$, $\Phi(p)$ and $\Psi(p)$ sufficiently smooth functions defined in $\Omega$ and on $S$.

Let us also define, for two points $p = (x_p, y_p, z_p)$ and $q = (x_q, y_q, z_q)$ in $\Omega$, the function $G(p, q)$, called the (free-space) Green’s function, such that:

$$G(p, q) = \frac{1}{4\pi k |p - q|} = \left(\frac{4\pi k r}{r}\right)^{-1}, \quad (2.9)$$

where $r$ is the Euclidean distance between $p$ and $q$, given by:

$$r = |p - q| = \left((x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2\right)^{\frac{1}{2}}. \quad (2.10)$$

The function $G(p, q)$ is the potential induced in a point $p$ due to a unit point charge placed in a point $q$ in a medium with uniform permittivity. From the definition of $G(p, q)$ we see that $G$ for $p \neq q$ satisfies the following equation:

$$\nabla^2 G(p, q) = 0, \quad (2.11)$$

and for $p = q$ is singular. These two properties of the Green’s function can be expressed as one equation:

$$k \nabla^2 G(p, q) = -\delta_q(p). \quad (2.12)$$

where $\delta_q(p)$ can be thought of as an infinitesimal (cylindrical) tower around the point $q$ of unit weight.

The first Green’s theorem for any fields $\Phi$ and $\Psi$ states that:

$$\int_{q \in \Omega} \Phi(q) \nabla^2 \Psi(q) \, dq = \int_{q \in S} \Phi(q) \frac{\partial \Psi(q)}{\partial n_q} \, dq - \int_{q \in \Omega} \nabla_q \Phi(q) \nabla_q \Psi(q) \, dq. \quad (2.13)$$

Interchanging $\Phi$ with $\Psi$ in Equation (2.13) produces another version of the theorem:

$$\int_{q \in \Omega} \Psi(q) \nabla^2 \Phi(q) \, dq = \int_{q \in S} \Psi(q) \frac{\partial \Phi(q)}{\partial n_q} \, dq - \int_{q \in \Omega} \nabla_q \Psi(q) \nabla_q \Phi(q) \, dq. \quad (2.14)$$

Subtracting side by side Equations (2.13) and (2.14) gives:

$$\int_{q \in \Omega} [\Phi(q) \nabla^2 \Psi(q) - \Psi(q) \nabla^2 \Phi(q)] \, dq = \int_{q \in S} [\Phi(q) \frac{\partial \Psi(q)}{\partial n_q} - \Psi(q) \frac{\partial \Phi(q)}{\partial n_q}] \, dq, \quad (2.15)$$
2.2 Boundary integral formulation

since

\[ \int_{q \in \Omega} \nabla_q \Phi(q) \nabla_q \Psi(q) \, dq = \int_{q \in \Omega} \nabla_q \Psi(q) \nabla_q \Phi(q) \, dq. \]  \hspace{1cm} (2.16)

Equation (2.15) expresses the second Green's theorem which often is called the "reciprocal version" of the Green's theorem.

The third Green's theorem describes the relation between \( \nabla_q^2 \Phi(q) \) in \( \Omega \) and the quantities \( \Phi(q) \) and \( (n_q \cdot \nabla_q \Phi(q)) \) on \( S \). This relation depends on the location of the point \( p \). Therefore, we distinguish the following three cases:

(i) \( p \in \Omega \);
(ii) \( p \in S \);
(iii) \( p \notin (\Omega \cup S) \).

To derive the third Green's theorem for the bounded region we start off with the second Green's theorem, which for \( \Phi(q) \) and \( \Psi(q) = G(p, q) \) states that:

\[ \int_{q \in \Omega} \left[ \Phi(q) \nabla_q^2 G(p, q) - G(p, q) \nabla_q^2 \Phi(q) \right] \, dq = - \int_{S} \left[ \Phi(q) \frac{\partial G(p, q)}{\partial n_q} - G(p, q) \left( \frac{\partial \Phi(q)}{\partial n_q} - \Phi(q) \frac{\partial G(p, q)}{\partial n_q} \right) \right] \, dq. \]  \hspace{1cm} (2.18)

It is obvious that for \( p \) lying inside \( \Omega \) or on \( S \) the Green's function is singular in the domain of integration. Thus for (i) and (ii) in (2.17) we use a special technique in which the neighborhood of the point \( p \) is excluded from the integration. The final expressions are obtained by taking the limits and observing that the integrals which appear in (2.18) are convergent.

Hence:

(i) for \( p \) inside \( \Omega \)

\[ \Phi(p) = - \int_{q \in \Omega} k G(p, q) \nabla_q^2 \Phi(q) \, dq \]
[\[ + \int_{q \in S} k [G(p, q) \frac{\partial \Phi(q)}{\partial n_q} - \Phi(q) \frac{\partial G(p, q)}{\partial n_q}] \, dq; \] \hspace{1cm} (2.19)]

(ii) for \( p \) on \( S \)

\[ \frac{1}{2} \Phi(p) = - \int_{q \in \Omega} k G(p, q) \nabla_q^2 \Phi(q) \, dq \]
[\[ + \int_{q \in S} k [G(p, q) \frac{\partial \Phi(q)}{\partial n_q} - \Phi(q) \frac{\partial G(p, q)}{\partial n_q}] \, dq; \] \hspace{1cm} (2.20)]

(iii) for \( p \) outside \( S \)

\[ 0 = - \int_{q \in \Omega} k G(p, q) \nabla_q^2 \Phi(q) \, dq \]
[\[ + \int_{q \in S} k [G(p, q) \frac{\partial \Phi(q)}{\partial n_q} - \Phi(q) \frac{\partial G(p, q)}{\partial n_q}] \, dq; \] \hspace{1cm} (2.21)]
2.2.2 Boundary integral formulation for an open domain

Until now we have dealt with the bounded domain $\Omega$, but for our modeling purposes we need to work with infinite (unbounded) $\Omega$. To derive an analogous third Green’s theorem for the unbounded domain we start off with the theorem formulated for the bounded domain.

Let us consider the configuration shown in Figure 2.1. The second Green’s theorem

\[
\int_{\partial \Omega} \left( \nabla \cdot \mathbf{H}(\mathbf{q}) \right) \cdot \mathbf{n} \, dS = -\int_{\Omega} \left( \nabla \times \mathbf{H}(\mathbf{q}) \right) \cdot \mathbf{E} \, dV.
\]

Figure 2.1. Extension of the boundary of a closed domain to infinity with $\Delta \to \infty$.

holds in the bounded domain lying outside $S$ but still inside $S_\Delta$. $S_\Delta$ is the surface of the sphere with the center in the observation point $p$ and with radius $\Delta$. We choose $\Delta$ so large that the surface $S$ lies entirely inside $S_\Delta$. Let $\Omega$ be a domain inside $S$ and $\Omega_\Delta$ the domain inside $S_\Delta$.

We assume that Laplace’s equation holds inside the domain $(\Omega_\Delta - \Omega)$:

\[
\nabla^2 \Phi(q) = 0 \quad \text{for } q \in (\Omega_\Delta - \Omega).
\]

Applying the third Green’s theorem for a bounded domain on the region $(\Omega_\Delta - \Omega)$ with the boundary which consists of $(S \cup S_\Delta)$, we obtain:

\[
\alpha \Phi(p) = -\int_{q \in (\Omega_\Delta - \Omega)} k G(p, q) \nabla_q^2 \Phi(q) \, dq
\]

\[
+ \int_{q \in (S \cup S_\Delta)} k \left[ G(p, q) \frac{\partial \Phi(q)}{\partial n_q} - \Phi(q) \frac{\partial G(p, q)}{\partial n_q} \right] \, dq.
\]
Here
\[
\alpha = \begin{cases} 
1 & \text{if } p \text{ is outside } S \\
\frac{1}{2} & \text{if } p \text{ is on } S \\
0 & \text{if } p \text{ is inside } S
\end{cases} \quad (2.24)
\]

The first volume integral on the right-hand side of (2.23) by assumption (2.22) equals zero, and the boundary integral evaluates to:
\[
\alpha \Phi(p) = \int_{q \in (S \cup S_{\Delta})} k[G(p, q)] \frac{\partial \Phi(q)}{\partial n_q} + \Phi(q) \frac{\partial G(p, q)}{\partial n_q} \, dq. \quad (2.25)
\]

We assume:

- all charges are concentrated in a sphere around the origin, as depicted in Figure 2.1;
- the Green's function and its gradient behave as:
  \[G(p, q) \sim O\left(\frac{1}{r}\right)\] and \[\nabla_q G(p, q) \sim O\left(\frac{1}{r^2}\right),\] with \[r = \frac{1}{|p-q|}.\]

Then, also \(\Phi(p) \sim O\left(\frac{1}{r}\right)\) and \(\nabla_p \Phi(p) \sim O\left(\frac{1}{r^2}\right),\) by the general relation connecting all charges (bound and free) to the field, see Equation (1.10), and the fact that all these charges are localized close to the origin.

Hence, the surface integral over \(S_{\Delta}\) becomes negligible:
\[
\int_{q \in S_{\Delta}} G(p, q) \frac{\partial \Phi(q)}{\partial n_q} \, dq \sim O\left(\frac{1}{\Delta} \cdot \frac{1}{\Delta^2} \cdot \Delta^2\right) = O\left(\frac{1}{\Delta}\right), \quad (2.26)
\]
and
\[
\int_{q \in S_{\Delta}} \Phi(q) \frac{\partial G(p, q)}{\partial n_q} \, dq \sim O\left(\frac{1}{\Delta} \cdot \frac{1}{\Delta^2} \cdot \Delta^2\right) = O\left(\frac{1}{\Delta}\right). \quad (2.27)
\]

The Green's function and further Green's functions which we will consider in later sections will all decay quickly enough at infinity to make integrals with infinite domains convergent. Although this point might give mathematical difficulties, in the case considered here there are no problems with convergence and the question has been well dealt with in the literature [Weber 54], [Hoop 75].

Taking into account the properties of \(\Phi\) and \(G\) when \(\Delta \to \infty\) and using the Green's formulation for the bounded region we obtain the following integral equation:
\[
\alpha \Phi(p) = \int_{q \in S} k[G(p, q)] \frac{\partial \Phi(q)}{\partial n_q} - \Phi(q) \frac{\partial G(p, q)}{\partial n_q} \, dq, \quad (2.28)
\]
with \(\alpha \) given by (2.24).

Later in this chapter we will derive a specialized Green's function for an unbounded layered medium. In this case Green's theorem with a multi-layer Green's function
must be slightly modified by taking into account the dielectric permittivity at the point \( q \):

\[
\alpha \Phi(p) = \int_{q \in S} \left[ G(p, q) k(q) \frac{\partial \Phi(q)}{\partial n_q} - k(q) \Phi(q) \frac{\partial G(p, q)}{\partial n_q} \right] dq,
\]

(2.29)

where \( k(q) \) is the constant dielectric permittivity of the layer in which a point \( q \) is located. The expression \( k(q) \frac{\partial \Phi(q)}{\partial n_q} \) denotes the charge density \( \sigma(q) \) on conductors.

### 2.2.3 Boundary integral formulation on an equipotential surface

Let us consider the boundary integral formulation for an open dielectric domain with constant permittivity as is given by Equation (2.28). Let us define the surface \( S \) as the union of \( N \) individual surfaces \( S = S_1 \cup S_2 \ldots \cup S_N \). Each of the individual conductor surfaces \( S_i \) acts like an equipotential. Equation (2.28) with Gauss’s law applied on the conductor surface yields:

\[
\frac{1}{2} \Phi(p) + \int_{q \in S} k(q) \frac{\partial G(p, q)}{\partial n_q} dq = \int_{q \in S} G(p, q) \sigma(q) dq.
\]

(2.30)

Assume that we wish to find \( \Phi(p) \) for some point \( p \) outside or on the conductor surface. For \( p \) in the domain \( \Omega \) the coefficient \( \alpha \) in Equation (2.28) equals 1. The case with \( p \) on the conductor boundary is troublesome. We overcome the difficulties in this case by taking a point \( p \) infinitely close to the surface of conductor, but staying in \( \Omega \). The Equation (2.28) can then be written as:

\[
\phi(p) + \int_{q \in S} k(q) \frac{\partial G(p, q)}{\partial n_q} dq = \int_{q \in S} G(p, q) \frac{\partial \Phi(q)}{\partial n_q} dq.
\]

(2.31)

Let us consider the integral on the left-hand side of Equation (2.31) which contains the normal derivative of the Green’s function:

\[
\int_{q \in S} k(q) \frac{\partial G(p, q)}{\partial n_q} dq.
\]

(2.32)

Since we know that \( \Phi(q) \) is constant over each conductor, we can split expression (2.31) and take the potential of the \( i \)th conductor \( \Phi_i \) out of the integral, which yields:

\[
\int_{q \in S} k(q) \frac{\partial G(p, q)}{\partial n_q} dq = \sum_{i=1}^{N} \Phi_i \int_{q \in S_i} k(q) \frac{\partial G(p, q)}{\partial n_q} dq.
\]

(2.33)

Since \( \frac{\partial G(p, q)}{\partial n_q} \) represents the normal component of the electrical field due to a unit point charge in \( q \) and the integral is over a closed surface, it represents the total charge within the conductor, which is simply zero.

Hence, we conclude that the integral (2.32) is zero and Equation (2.31) evaluates to:

\[
\Phi(p) = \int_{q \in S} G(p, q) (k \frac{\partial \Phi(q)}{\partial n_q}) dq
\]

(2.34)

as desired.
2.3 The boundary element method in capacitance modeling

2.3.1 Boundary integral formulation

Consider a geometry consisting of a number of ideal conductors embedded in a perfectly stratified dielectric medium for which the prime integrals in the form of the Green's function are known.

Before going into details, which we postpone to Chapter 4, we assume additionally for the purpose of hybrid modeling that the other conducting bodies can be embedded in the dielectric medium, but do not behave as ideal conductors. We assume that the charge accumulates on their surface (no charge inside) but their surface is not equipotential. In this chapter we call them "conductors" as well. In later chapters we will distinguish these conducting bodies from ideal conductors.

Let:

- be the real potential at a point \( p \),
- \( \Phi(p) \) be the approximate potential at a point \( p \),
- \( k(p) \) be the dielectric permittivity at a point \( p \),
- \( \frac{\partial}{\partial n_q} \) be the derivative along the outward normal \( n_q \) to the surface \( S(q) \),
- \( \sigma(q) = k(q) \frac{\partial k(q)}{\partial n_q} \) be the charge density along \( S(q) \),
- \( S_c \) denotes all charged surfaces in the system.

Since conducting surfaces which are not equipotential exist in the system, we cannot use the simplified boundary integral Equation (2.34), which is based on the equipotential property of ideal conductors. We have to make one step back before this simplification, and we use the boundary integral Equation (2.30) which includes the term containing the integral of the normal derivative of the Green's function.

The electrostatic potential at the point \( p \), which lies on a conductor, generated by a charge of conductors in an otherwise chargeless 3D stratified dielectric satisfies the boundary integral equation obtained by using the Green’s theorem:

\[
\frac{1}{2} \Phi(p) + \int_{q \in S_c} \Phi(q) k(q) \frac{\partial G(p,q)}{\partial n_q} \, dq = \int_{q \in S_c} G(p,q) \sigma(q) \, dq
\]

Here, \( \sigma(q) \) denotes the exact charge density on the conductor surface.

2.3.2 Discretization

The reduction of the integral Equation (2.35) to a discrete form requires the piecewise-discretization of the charge on conductors in the medium. Since the charge is essentially concentrated on the surface of the conductors, only the surface needs to be discretized.
We partition the conductor surface into a number, say \( N \), triangular sub-domains called boundary elements:

\[
S_c = \bigcup_{j=1}^{N} S_j
\]  

(2.36)

Hence every boundary integral defined over the surface \( S_c \) can be expressed in terms of independent integrals over boundary elements. Therefore the boundary integral equation given by (2.35) can be rewritten as:

\[
\frac{1}{2} \Phi(p) + \sum_{j=1}^{N} \left[ \int_{q \in S_j} \Phi^j(q) k(q) \frac{\partial G(p, q)}{\partial n_q} \, dq \right] = \sum_{j=1}^{N} \left[ \int_{q \in S_j} G(p, q) \sigma^j(q) \, dq \right],
\]  

(2.37)

where \( \Phi^j(q) \) and \( \sigma^j(q) \) in the integrands may be approximated by means of interpolation expressions in terms of their values at some nodes defined on the \( j^{th} \) element. There are many ways to accomplish the discretization of these quantities.

### 2.3.3 Shape functions

The key problem of discretization is how the potential \( \Phi \) and the charge density \( \sigma \) are approximated by means of interpolation expressions in terms of their values at some nodes defined over the element. Extensive discussion of the various types of interpolation expressions can be found in textbooks on elastostatics, mechanics and fluid flow etc., e.g., [Fletcher 84], [Burnett 88].

Many researchers, working on capacitance extraction, have been using various types of approximating functions, with different results. Let us recall, for example, piecewise constant approximation of the charge density used in [Patel 71], [Ruehli 73], or non-constant approximation presented in [Benedek 72], [Balaban 73].

We can basically consider the approximation problem in the following four aspects:

- choice of "planar" or "curved" elements;
- choice of the shape of the boundary elements;
- choice of the node placement over the element;
- choice of the (interpolation) shape function in the element.

The difference between the "planar" and "curved" elements is displayed in Figure 2.2. The "curved" elements model the boundaries more precisely than the "planar" ones, but they require more computational effort due to the use of a parametric mapping.
2.3 The boundary element method in capacitance modeling

Figure 2.2. Examples the different types of elements: (a) planar, (b) curved.

After we decide to use "planar" elements, with reference to the second criterion we can choose between triangles, quadrilaterals, etc. These "regularly" shaped elements can always be translated by means of a parametric mapping into "curved" elements. In Figure 2.3 we show the parent element, which is the triangular "planar" element, and the "curved" element obtained by a relevant mapping.

Figure 2.3. Parametric mapping onto a "curved" element; (a) the parent "planar" element, (b) the "curved" element showing the parent element mapped onto it.

Usually the parent triangle is a right-angled triangle because two of the sides can then be aligned with the Cartesian $x, y$-axes, simplifying the complexity of the algebra for the mapping.

The next criterion considers the node placement in the element. There exist many families of elements based on this criterion. As an example we recall only two: the Lagrange family and the serendipity family for quadrilateral elements. We show the first few elements of both families in Figure 2.4. The serendipity family of
rectangular elements can be obtained by taking the Lagrange shape functions for these elements and modifying them to eliminate the internal nodes of these element. The terms contributing to the interpolation functions can be collected in an array called Pascal's triangle, as shown in Figure 2.5.

![Figure 2.4. First four elements of: (a) the Lagrange family and (b) the serendipity family.](image)

![Figure 2.5. Terms contributing to the approximating function.](image)

We can see that every term has the form $x^k y^l$, where $k, l = 0, 1, \ldots$. The degree of the term is the sum of $k$ and $l$. The highest degree of all terms in the polynomial is the degree of approximation. There are two ways of increasing accuracy of the approximation:
2.3 The boundary element method in capacitance modeling

1. to increase the number of elements while using the same kind of approximation in the element;

2. to keep the number of elements (the same size) while increasing the degree of the interpolation functions in each element.

It has been observed that the number of contributing nodes in an algebraic equation increases rapidly with the increase of the degree of the interpolation function. This, of course, causes a significant increase in execution time. One must then choose between the two options.

We base our choice on the following criteria:

- execution time;
- accuracy of the solution.

The lower order approximating functions such as constant and linear shape functions provide good approximations and demand less of computational effort than what is needed for higher order shape functions. Moreover, lower order shape functions allow us to perform analytical calculation of the integrals which appear in the boundary integral equations. The last property is quite important since this improves the numerical performance of the method. We will show later that this allows us to tackle singular integrals in a highly efficient way.

Taking into account the above considerations we decide to use constant shape functions which provide a piecewise constant distribution of the charge density on the charged surfaces.

2.3.4 Piecewise constant approximation of the charge density

We assume that the charge density has an average constant value over each boundary element attached to the center of gravity of the element. Thus, for each $i^{th}$ boundary element the charge $\sigma_i$ is assigned to the node lying at the center of gravity of the $i^{th}$ element. The discretization of the potential follows. We have the element potential $\Phi_i$ attached to the same node on the element.

For a conductor mesh consisting of $N$ triangular boundary elements, the charge density is then approximated as:

$$\sigma(q) \approx \tilde{\sigma}(q) = \sum_{i=1}^{N} \sigma_i f_i(q).$$  \hspace{1cm} (2.38)

The function $f_i(q)$, defined on the $i^{th}$ boundary element, is called a shape function and has the following properties:

1. It is non-zero only on the $i^{th}$ triangular boundary element with area $S_i$;
2. It is normalized as follows:

\[
\int_{q \in S_j} f_i(q) \, dq = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j.
\end{cases}
\]  

(2.39)

In the case of charges on a conductor we take \( f_i(q) \) to be constant, thus:

\[
f_i(q) = \begin{cases} 
\frac{1}{S_i} & \text{for } q \in S_i \\
0 & \text{otherwise}.
\end{cases}
\]  

(2.40)

This results in the piecewise constant charge distribution over the surface of the conductor, as illustrated in Figure 2.6.

Hence, \( \sigma^j(q) \) as used in Equation (2.37) can be expressed as:

\[
\sigma^j(q) = \sigma_j f_j(q)
\]  

(2.41)

for the \( j^{th} \) element. From this it follows that the potential \( \Phi^j(q) \) in the left-hand side integral can be expressed as:

\[
\Phi^j(q) = \Phi_j,
\]  

(2.42)

with \( \Phi_j \) the average value over the \( j^{th} \) element.

Substituting (2.41) and (2.42) into (2.37) we arrive at the discretized boundary element equation on the conductor surface:

\[
\frac{1}{2} \Phi(p) + \sum_{j=1}^{N} \Phi_j \left[ \int_{q \in S_j} k(q) \frac{\partial G(p, q)}{\partial n_q} \, dq \right] = \sum_{j=1}^{N} \sigma_j \left[ \int_{q \in S_j} G(p, q) f_j(q) \, dq \right],
\]  

(2.43)

Here \( \Phi(p) \) denotes the approximate solution for the potential. It can be shown that the method (under reasonable assumptions) produces an approximation of \( O(h) \) for the potential, where \( h \) is the size of the mesh element.
2.3 The boundary element method in capacitance modeling

2.3.5 The Galerkin method

It is obvious that, in order to solve for \( N \) unknown \( \sigma_j \)'s, we need to construct \( N \) independent equations. These can be derived using the so-called Galerkin method which is one of the types of weighted residual methods (WRM) [Mikhlin 67], [Harrington 68], [Benedek 72], [Burnett 88].

The method of weighted residuals is a general method of obtaining solutions to partial differential equations. The unknown solution is expanded in a set of approximating functions, which are specified, but with adjustable constants which are chosen to give the best solution to the differential equation.

We search for the potential \( \Phi(p) \) that satisfies the second order differential equation – the Laplace’s equation:

\[
\nabla_p [k(p) \nabla_p \Phi(p)] = 0. \tag{2.44}
\]

Substitution of an approximate solution \( \hat{\Phi}(p) \) into the Laplace equation results in a non-zero function which we call the residual \( R(p) \):

\[
R(p) = \nabla_p [k(p) \nabla_p \hat{\Phi}(p)] \neq 0. \tag{2.45}
\]

The approximate solution is then expressed in terms of the coefficients \( \sigma_j \) and the interpolation (shape) functions:

\[
\hat{\Phi}(p) = F(\sigma_1, \sigma_2, ..., \sigma_N; f_1(p), f_2(p), ..., f_N(p)). \tag{2.46}
\]

The WRM sets the following inner product equal to zero in order to find the \( \sigma_j \)'s:

\[
< R(p), w_i(p) > = 0, \quad i = 1, 2, ..., N, \tag{2.47}
\]

where the \( w_i \)'s are the weighting functions.

The inner product is defined as:

\[
< R(p), w_i(p) > = \int_{p \in \Omega} R(p) w_i(p) \, dp. \tag{2.48}
\]

If the weighting functions form a complete set of functions, then Equation (2.47) says that residual \( R(p) \) must be orthogonal to every member of the complete set of weighting functions. This implies that for \( N \to \infty \) the residual \( R(p) \) converges to zero in the mean, this property is called weak convergence, see for references [Mikhlin 67] and [Gohberg 74]. Now, if \( R(p) \) converges to zero in the mean and the approximate solution satisfies the boundary conditions exactly, then the approximate solution converges to the exact solution in the mean too.

We use the theory of the WRM presented above again in Chapter 3, in which we discuss the finite element method. For the purpose of the boundary element method we have to adapt the theory of WRM, developed for the partial differential equations, to the integral equations.
The Boundary Element Method

The Green's theorem allows us to reduce the differential equation to the boundary equation from which we can derive the expression for the potential $\Phi(p)$. Thus instead of working with the residual defined by (2.45) we work with the solution residual error $E(p)$ which is defined as:

$$ E(p) = \Phi(p) - \tilde{\Phi}(p) \tag{2.49} $$

The approximate potential $\tilde{\Phi}(p)$ is expressed in terms of the approximate charge density on the surface of conductors given as:

$$ \tilde{\sigma}(q) = \sum_{i=1}^{N} \sigma_i f_i(q) \tag{2.50} $$

To find a good approximation for the potential one must find the coefficients $\sigma_i$'s. To determine the $N$ unknown $\sigma_i$ coefficients one needs to formulate $N$ independent equations using independent weighting functions.

The WRM enforces the error $E(p)$ to be zero in the average sense over the entire domain of $\Phi(p)$, the surface of conductors. Since the potential is expressed in terms of the approximate boundary charge on the conductors, we need to average the solution error only there. Therefore, we demand the inner product of the error $E(p)$ with each function from the set of the weighting functions $\{w_i(p)\}_{i=1}^{N}$ to be zero, namely:

$$ < E(p), w_i(p) > = \int_{p \in \Omega} E(p)w_i(p) \, dp = 0, \quad \text{for} \quad i = 1, ..., N. \tag{2.51} $$

Various types of weighting functions can be used. Each of them leads to a different weighted residual approximation method. Depending on the weighting functions being used, we distinguish [Brebbia 78], [Burnett 88], [Zienkiewicz 83]:

1. the point collocation method;
2. the sub-domain method;
3. the least-squares method;
4. the Galerkin method.

The Galerkin method [Mikhlin 67] makes a convenient choice of the weighting functions. They are the same as the approximating shape functions:

$$ w_i(p) = f_i(p). \tag{2.52} $$

For each parameter in an approximating solution we require that the weighted “average” of the residual error over the entire domain to be zero:

$$ < \Phi(p) - \tilde{\Phi}(p), f_i(p) > = 0 \quad \text{for} \quad i = 1, ..., N. \tag{2.53} $$
And again we obtain a system of $N$ residual equations.

Galerkin's method requires Equation (2.53) to be true over the set of the shape functions in use. The left linearity of the inner product $<.,.>$ allows us to write Equation (2.53) as:

$$<\Phi(p), f_i(p) > = <\Phi(p), f_i(p) > \text{ for } i = 1, \ldots, N.$$  \hspace{1cm} (2.54)

We consider first the right-hand side of Equation (2.54). Substituting (2.43) into the right-hand side of Equation (2.54) we obtain:

$$2 <\Phi(p), f_i(p) > = 2 \sum_{j=1}^{N} \sigma_j \left[ \int_{q \in S_j} G(p, q) f_j(q) \, dq \right]$$

$$- \sum_{j=1}^{N} \Phi_j \left[ \int_{q \in S_j} k(q) \frac{\partial G(p, q)}{\partial n_q} \, dq \right] f_i(p) >$$

$$= 2 \sum_{j=1}^{N} \sigma_j \left[ \int_{p \in S_j} \int_{q \in S_j} G(p, q) f_j(q) f_i(p) \, dq \, dp \right]$$

$$- \sum_{j=1}^{N} \Phi_j \left[ \int_{p \in S_j} \int_{q \in S_j} k(q) \frac{\partial G(p, q)}{\partial n_q} \, f_i(p) \, dq \, dp \right], \hspace{1cm} (2.55)$$

for all $i = 1, \ldots, N$.

The left-hand side of Equation (2.54) evaluates to:

$$<\Phi(p), f_i(p) > \text{ for } i = 1, \ldots, N.$$  \hspace{1cm} (2.56)

We have assumed before, that $\Phi^i(p) = \Phi_i$ is an average constant value over the $i$th element attached to the only node representing the element, namely the center of gravity of the $i$th element. The smallness of the element is essential. We assume that for elements small enough the potential varies only slightly over the element. Then we may use the mean value theorem which says that for some point $\xi_i$ located on the $i$th element the value of potential $\Phi(\xi_i)$ is bounded by the smallest and the largest value of the potential on the element. We choose the point $\xi_i$ to be the center of gravity of the $i$th element. Since the shape function $f_i(p)$ is normalized over the $i$th element, Equation (2.56) becomes:

$$<\Phi(p), f_i(p) > = \int_{p \in S_i} \Phi_i f_i(p) \, dp = \int_{p \in S_i} \Phi_i f_i(p) \, dp = \Phi_i,$$  \hspace{1cm} (2.57)

here $\Phi_i$ is the average constant (mean) value of the potential over the $i$th element.

Substitution of (2.55) and (2.57) into Equation (2.54) yields:

$$\frac{1}{2} \Phi_i + \sum_{j=1}^{N} \Phi_j \left[ \int_{p \in S_j} \int_{q \in S_j} k(q) \frac{\partial G(p, q)}{\partial n_q} \, f_i(p) \, dq \, dp \right] =$$

$$\sum_{j=1}^{N} \sigma_j \left[ \int_{p \in S_j} \int_{q \in S_j} G(p, q) f_j(q) f_i(p) \, dq \, dp \right] \text{ for } i = 1, \ldots, N. \hspace{1cm} (2.58)$$
For:

- \( \Phi = [\Phi_1, \Phi_2, \ldots, \Phi_N]^T \) and \( \sigma = [\sigma_1, \sigma_2, \ldots, \sigma_N]^T \) the element potentials and charges, respectively;
- \( G^{(n)} \) the matrix with entries:
  \[
  G^{(n)}_{ij} = \int_{p \in S_i} \int_{q \in S_j} k(q) \frac{\partial G(p, q)}{\partial n_q} f_i(p) \, dq \, dp;
  \]  
  \( (2.59) \)
- \( G \) the matrix with entries:
  \[
  G_{ij} = \int_{p \in S_i} \int_{q \in S_j} G(p, q) f_i(p) f_j(q) \, dq \, dp;
  \]  
  \( (2.60) \)
- \( I \) the identity matrix;

Equation (2.58) converts to a matrix form as:

\[
\left[ \frac{1}{2} I + G^{(n)} \right] \Phi = G \sigma
\]  
\( (2.61) \)

**Short-circuit capacitance matrix**

In this section we are concerned only with ideal conductors.

From Equation (2.61) follows an expression for the element capacitance matrix:

\[
C_c = G^{-1} \left[ \frac{1}{2} I + G^{(n)} \right]
\]  
\( (2.62) \)

It turns out that the matrix \( C_c \) as given in Equation (2.62) is not intrinsically symmetric. This is, however, due to the discretization. One can show that \( C_c \) is almost symmetric (the system is passive and conserves the energy, see [Weber 54]).

The final value is obtained by symmetrization:

\[
C = \frac{1}{2} [C_c + C_c^T].
\]  
\( (2.63) \)

Here \( C \) is a matrix representing a model consisting of capacitances between each pair of boundary elements. Thus our element-wise model is described by:

\[
C \Phi = \sigma.
\]  
\( (2.64) \)

To derive the multiconductor capacitances, which is our ultimate goal, we have to establish the incidence between the boundary elements and the conductors. To do so we use the incidence matrix \( A \). The matrix \( A \) is a rectangular \( N \times M \) matrix.
2.4 Multiconductor capacitances

where $N$ denotes the total number of boundary elements in the system, and $M$ denotes the number of conductors. $A$ is such a matrix that:

$$A_{ij} = \begin{cases} 1 & \text{if } i^{th} \text{ element lies on } j^{th} \text{ conductor} \\ 0 & \text{otherwise} \end{cases} \quad (2.65)$$

Moreover, let $V = [V_1 V_2 ... V_M]^T$ be the vector of conductor potentials and $Q = [Q_1 Q_2 ... Q_M]^T$ the vector of charges on conductors. We recall that the charge on a conductor is the sum of all elemental charges on that conductor, which we write as:

$$Q = A^T \sigma. \quad (2.66)$$

Furthermore, the element potentials are the same for all elements on an ideal conductor, since the conductor forms an equipotential. This can be expressed as:

$$\Phi = AV. \quad (2.67)$$

The following derivation is valid:

$$Q = A^T \sigma = A^T C \Phi = A^T C A V = C_s V, \quad (2.68)$$

where $C_s = A^T C A$ is the short-circuit capacitance matrix.

2.4 Multiconductor capacitances

2.4.1 The short-circuit capacitance matrix

Formula (1.13) expresses an important relationship in the modeling of the interconnect capacitances. Our goal is the calculation of the inverse of the elastance matrix $G$, which is the capacitance matrix that relates the total charges on the conductors to their various potentials, or in other words, to determine the charge on each conductor when the electrostatic potential is specified at each conductor.

The principle of superposition allows the charge on the $i^{th}$ conductor to be written in terms of the applied potentials as:

$$Q_i = \sum_{j=1}^{N} C_{sij} \Phi_j, \quad (2.69)$$

where the $C_{sij}$'s are called the coefficients of capacitance, and $N$ is the number of conductors in the system.

Referring to Figure 1.2, we express the charge $Q_i$ on the $i^{th}$ conductor as a function of the three conductor voltages $V_i$ (for $i = 1, 2, 3$) by:

$$\begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \end{bmatrix} = \begin{bmatrix} C_{s11} & C_{s12} & C_{s13} \\ C_{s21} & C_{s22} & C_{s23} \\ C_{s31} & C_{s32} & C_{s33} \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \end{bmatrix}. \quad (2.70)$$
The matrix $C_s$ which appears in Equation (2.70) is called the short-circuit capacitance matrix of the conductor system. The $C_s$ matrix owes its name to the fact that the entry $C_{sij}$ is related to the charge on conductor $i$ when the conductor $j$ is maintained at unit potential and all other conductors are short-circuited to the ground (i.e. are held at zero potential), e.g.:

$$C_{s12} = \frac{Q_1}{V_2} | v_1 = v_2 = 0.$$  \hspace{1cm} (2.71)

### 2.4.2 Properties of the short-circuit capacitance matrix

The entries of the $C_s$ matrix are strictly dependent on the geometry of the conductors and the dielectric structure of the IC. The calculation of these values is quite involved, but even then before their evaluation we can predict many of the properties of the short-circuit capacitance matrix based on the physical principles.

First, using the Green's theorem, it can be shown that the capacitance matrix $C_s$ is symmetric:

$$C_{sij} = C_{sji}. \hspace{1cm} (2.72)$$

This follows also from energy conservation, see [Weber 54].

Second, the main diagonal entries of the $C_s$ matrix are positive and the off-diagonal entries are negative. Suppose that the $i^{th}$ conductor is held at some positive voltage while the other conductors are grounded (held at zero potential). In order to ensure that the $i^{th}$ conductor is held at a positive voltage, the charge carried by this conductor must be positive too. Thus we can conclude that:

$$C_{sii} > 0. \hspace{1cm} (2.73)$$

The other conductors which are kept at zero voltage must carry negative charges. Thus,

$$C_{sij} < 0 \quad \text{for} \quad i \neq j. \hspace{1cm} (2.74)$$

Third, the short-circuit capacitance matrix is positive definite. The total energy of the system of $N$ conductors can be expressed as [Weber 54], [Ruehli 87]:

$$\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} V_i C_{sij} V_j. \hspace{1cm} (2.75)$$

The total electrostatic energy of the system of conductors must be greater than zero, for all cases in which at least one conductor is at non-zero voltage, because work is required to assemble any non-zero charge distribution. To ensure this physical property the $C_s$ matrix must be positive definite.
Fourth, and finally, the $C_s$ matrix is strictly diagonally dominant. We say that the matrix is strictly diagonally dominant if the following condition is satisfied:

$$C_{sii} > \sum_{j \neq i} |C_{sij}|.$$ \hspace{1cm} (2.76)

To show that the $C_s$ matrix satisfies this requirement let us consider the situation in which all conductors in the system are held at unit voltage $V_u$. Since all conductors are at the same voltage there are no field lines going between the conductors. The only field lines which exist in the described system originate on positively charged conductors and terminate at infinity. Substituting $V_i = V_u$ for all $i$'s, into Equation (2.69) we obtain:

$$Q_i = \sum_{j=1}^{N} C_{sij} V_u > 0.$$ \hspace{1cm} (2.77)

Since $C_{sii} > 0$, and $C_{sij} < 0$ for $i \neq j$, the property given by Equation (2.76) follows from (2.77).

### 2.4.3 Network interpretation of the short-circuit capacitance matrix

The short-circuit capacitance matrix, as given by (2.70), describes an equivalent lumped network which consists of two types of capacitances: the coupling capacitances between different conductors and the autocapacitances between each conductor and the reference – the ground plane.

In order to explain the concept of the coupling and ground capacitances let us first consider the simplest case of two conductors above the ground plane, as shown in Figure 2.7.

![Figure 2.7](image)

**Figure 2.7.** Field lines in a two conductor system above the ground plane.
In such a configuration, the first conductor is carrying the charge $Q_1$:

$$Q_1 = Q_{1g} + Q_{12}$$  \hspace{1cm} (2.78)

and the second conductor the charge $Q_2$:

$$Q_2 = Q_{2g} + Q_{21}$$  \hspace{1cm} (2.79)

We can define the following capacitances in the system:

$$C_{1g} = \frac{Q_{1g}}{V_1 - V_g}$$  \hspace{1cm} (2.80)

$$C_{12} = \frac{Q_{12}}{V_1 - V_2}$$  \hspace{1cm} (2.81)

$$C_{2g} = \frac{Q_{2g}}{V_g - V_2}$$  \hspace{1cm} (2.82)

and because of the distribution displayed in Figure 2.7 we can conclude that $C_{1g} = C_{g1}, C_{12} = C_{21}, C_{g2} = C_{2g}$. The capacitance $C_{12}$ is called the coupling capacitance, $C_{1g}$ and $C_{2g}$ are called the ground capacitances of the first and second conductor, respectively.

From Equations (2.78–2.82) we derive the following set of equations:

$$Q_1 = C_{1g} (V_1 - V_g) + C_{12} (V_1 - V_2)$$

$$Q_2 = C_{2g} (V_2 - V_g) + C_{21} (V_2 - V_1)$$  \hspace{1cm} (2.83)

For $V_g = 0$ and $C_{12} = C_{21}$ the set of equations (2.83) evaluates to:

$$\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} = \begin{bmatrix} (C_{1g} + C_{12}) & -C_{12} \\ -C_{12} & (C_{g2} + C_{12}) \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix}$$  \hspace{1cm} (2.84)

Of course the question appears how to couple the values of capacitors in the lumped network with the values of the entries of the $C_s$ matrix.

![Figure 2.8](image.png)

*Figure 2.8. Equivalent capacitive network for the system of three conductors.*
The network depicted in Figure 2.8 can be described by a set of linear equations in terms of the lumped capacitors as:

\[
\begin{align*}
Q_1 &= C_{11}V_1 + C_{12}(V_1 - V_2) + C_{13}(V_1 - V_3) \\
Q_2 &= C_{21}(V_2 - V_1) + C_{22}V_2 + C_{23}(V_2 - V_3) \\
Q_3 &= C_{31}(V_3 - V_1) + C_{32}(V_3 - V_2) + C_{33}V_3
\end{align*}
\] (2.85)

where each \( C_{ij} \) for \( i \neq j \) is the coupling capacitance between the conductors \( i \) and \( j \), and \( C_{ii} \) is the ground capacitance of the conductor \( i \).

In fact, between the entries of the \( C \) matrix and the capacitance values appearing in the above set of linear equations, the following relationship holds:

\[
C_{sii} = \sum_{j=1}^{3} C_{ij} \quad \text{for} \quad i = 1, 2, 3 \quad (2.86)
\]

and

\[
C_{sij} = -C_{ij} \quad (2.87)
\]

\( C_{sii} \) denote the diagonal entries of \( C \), which are simply the sums of the ground and coupling capacitances for each conductor \( i \).

### 2.5 Green’s function

In the previous sections we have discussed the applicability of the Green’s function for capacitance extraction. In order to solve the capacitance modeling problem one may work with the free space Green’s function and the bound charge at the dielectric interfaces or to develop the specialized Green’s function for multilayered dielectric media. In general, the construction of the specialized Green’s function might not be easy. A number of approaches to determine the Green’s function for multilayered dielectric media have been developed. Among them, especially popular are:

- the method of images;
- the expansion into orthogonal functions;
- the separation of variables.

We will briefly discuss each of the above methods followed by a more detailed presentation of our method, starting at Section 2.5.5. To make the presentation of these methods complete, we also include a brief discussion on the free space Green’s function and the bound charge.
2.5.1 Free space Green’s function and the bound charges at dielectric interfaces

Let us first consider the approach in which the bound charge is treated explicitly. The potential $\Phi(p)$ at any point $p$ of a dielectric medium is determined by all charges in free space according to the expression:

$$\Phi(p) = \int_{S_c \cup S_{di}} G(p, q) \sigma^T(q) \, dq,$$

(2.88)

with $S_c$ the surface of conductors and $S_{di}$ the surface of dielectric interfaces. We use here the concept of the total charge, according to which the total charge density $\sigma^T$ is:

$$\sigma^T = \sigma^B + \sigma^F,$$

(2.89)

where $\sigma^B$ is the bound charge at dielectric interfaces due to a discontinuity of the dielectric flux through these interfaces, and $\sigma^F$ is the free charge, i.e. the charge on the conductors.

We enforce as well two boundary conditions:

- the conductor surfaces are equipotential;
- the discontinuity of the normal component of the displacement field across the dielectric interfaces must be equal to the local bound charge density.

Combining discretized Equation (2.88) with these boundary conditions, one obtains the following matrix equation:

$$\begin{bmatrix} P_{FF} & P_{FB} \\ P_{BF} & P_{BB} \end{bmatrix} \begin{bmatrix} \sigma^F \\ \sigma^B \end{bmatrix} = \begin{bmatrix} \Phi \\ 0 \end{bmatrix},$$

(2.90)

Eliminating $\sigma^B$ from Equation (2.90) provides the relation between conductor charges and conductor potentials. The technique, which we have briefly presented, extends the size of the matrix relating the potentials and the charges by the additional number of charges at the dielectric interfaces. This larger size of the matrix implies a higher computational cost.

2.5.2 Method of images

The method of images is a technique to determine the Green’s function. The method is applicable to problems concerning one or more point charges in the presence of boundary surfaces (they might have different shapes, e.g. planes, spheres etc.). In this method, the point charges are distributed in space to satisfy the required boundary conditions. It is possible to deduce from a given geometry that a number of distributed charges of appropriate magnitudes can simulate the boundary conditions.
2.5 Green’s function

Figure 2.9. (a) Dielectric half plane with a point charge at the point \( q \). (b) The original point charge and its image in configuration with a half plane.

These charges are called **image charges**. The method is extensively discussed by Weber in his book [Weber 54].

From the point of view of capacitance extraction we are interested in layered structures. For such structures the method of images can be used to construct the Green’s function. As an example let us consider a dielectric half plane above the ground plane as shown in Figure 2.9(a). The method of images transforms the considered domain into a homogeneous domain with additional image charges. A system of point charges \( Q \) distributed above the ground plane is treated as a system without this plane, but with so-called “reflection” \( Q' \) of each point charge about the ground plane, and such that \( Q' = -Q \) in magnitude but has an opposite sign, see Figure 2.9(b).

If we assume that \( p \) and \( q \) are points with coordinates \((x_p, y_p, z_p)\) and \((x_q, y_q, z_q)\), respectively, we obtain the following specialized Green’s function:

\[
G(p, q) = \frac{1}{4\pi k} \left[ \frac{1}{\sqrt{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2}} - \frac{1}{\sqrt{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p + z_q)^2}} \right].
\]  

(2.91)

This expression can be simplified by the introduction of an auxiliary lateral distance \( r \) between \( p \) and \( q \):

\[
r = \sqrt{(x_p - x_q)^2 + (y_p - y_q)^2}
\]

(2.92)

Hence, Equation (2.91) can be written as:

\[
G(p, q) = \frac{1}{4\pi k} \left[ \frac{1}{\sqrt{r^2 + (z_p - z_q)^2}} - \frac{1}{\sqrt{r^2 + (z_p + z_q)^2}} \right].
\]

(2.93)

The second term in Equation (2.93) is considered to be a correction term, which is necessary when the ground plane is present. Otherwise if the ground plane is not
Let us first consider the approach in which the corrections of the form (2.93) are applied. The potential due to a point charge $q$ at the point $p$ of a medium with an interior ground plane is obtained by applying a correction to the free space potential $G(p, q)$.

The Green's function for any point lying inside the bottom layer with permittivity $k_1$ is given by the formula:

$$G_1(p, q) = \frac{1}{4\pi k_1} \left[ \frac{1}{\sqrt{r^2 + (z_p - z_q)^2}} - \frac{1}{\sqrt{r^2 + (z_p + z_q)^2}} \right] + \sum_{n=0}^{\infty} (-1)^n k^{(n+1)} \frac{1}{\sqrt{r^2 + [2(n+1)d - (z_p + z_q)]^2}}$$

Figure 2.10. (a) Two-layered dielectric medium with a point charge at the point $q$. (b) First few images of a point charge in the two-layered dielectric configuration. Here $K$ is a coefficient defined as $K = \frac{k_1 - k_2}{k_1 + k_2}$.
2.5 Green's function

\[
- \frac{1}{\sqrt{r^2 + [2(n + 1)d + (z_p - z_q)]^2}} \\
+ \frac{1}{\sqrt{r^2 + [2(n + 1)d + (z_p + z_q)]^2}} \\
- \frac{1}{\sqrt{r^2 + [2(n + 1)d - (z_p - z_q)]^2}}
\]

(2.95)

where \( k_1 \) and \( k_2 \) are the dielectric permittivities of the layers one and two, \( d \) is the thickness of the first layer and \( K = \frac{k_1 - k_2}{k_1 + k_2} \).

For multiple dielectrics the method of images leads to quite complex formulas with many nested infinite series. Practice shows that for more than three dielectric layers the method becomes unusable.

The problem of the determination of the Green’s function using the method of images becomes even more difficult for the finite bounded dielectrics. In this case the images are required to match the boundary conditions on the side faces of the dielectric medium too. This results in adding of more levels of nested summations in the formula for the Green’s function.

2.5.3 Expansion in orthogonal functions

The representation of the Green’s function by expansion in orthogonal functions is a powerful technique, which guarantees reasonably good convergence properties. Commonly used sets of orthogonal functions consist of sines and cosines, and expansion in terms of them is called a Fourier series. Detailed derivation of the Green’s function, for the bounded two-layered dielectric medium, by using Fourier expansion can be found in [Dewilde 90].

2.5.4 Separation of variables

The separation of variables technique is a classical tool for solving partial differential equations. The technique is based on the assumption that the potential can be represented as a product of functions which depend on a smaller number of coordinate variables than the potential function. The separation of variables technique has been discussed widely in [Weber 54] and [Jackson 75]. The potential, so the Green’s function as well, in the cylindrical coordinate system can be expanded in terms of Bessel functions. In spherical coordinates, the potential can be expanded in terms of Legendre polynomials.

2.5.5 Unbounded multilevel dielectric problem

To construct the Green’s function for an unbounded multilayered dielectric medium, we make a convenient choice of expansion of the Green’s function in terms of Bessel functions. Detailed derivation of the Green’s function for layered unbounded dielectric medium has been presented in [Weber 54], [Dewilde 90], [Meijs 94].
In general, the Green’s function for $N$ dielectric layers can be written as follows:

$$g_{ij}(z_p, z_q, r) = \frac{1}{4\pi k_j} \int_0^\infty \left( A_{ij} e^{m(z_p - z_q)} + B_{ij} e^{m(z_q - z_p)} + \delta_{ij} e^{-m|z_p - z_q|} \right) J_0(mr) \, dm. \quad (2.96)$$

Here, $m$ is a constant, $J_0$ denotes the Bessel function of first kind and zero order, $A_{ij}$ and $B_{ij}$ are the parameters which are determined by the boundary conditions.

The boundary conditions in force are as follows:

1. The potential vanishes at the ground plane and at infinity:
   $$g_{ij}(0, z_q, r) = 0 \quad j = 1, ..., N, \quad (2.97)$$
   $$g_{Nj}(\infty, z_q, r) = 0 \quad j = 1, ..., N. \quad (2.98)$$

2. The potential is continuous across each dielectric interface:
   $$g_{ij}(h_i, z_q, r) = g_{(i+1)j}(h_i, z_q, r) \quad i, j = 1, ..., N, \quad (2.99)$$
   here $h_i$ is the height of the $i^{th}$ dielectric interface above the ground plane.

3. The displacement field is continuous across each dielectric interface:
   $$k_j \frac{\partial g_{ij}(z_p, z_q, r)}{\partial z_p} \bigg|_{z_p = h_i} = k_{i+1} \frac{\partial g_{(i+1)j}(z_p, z_q, r)}{\partial z_p} \bigg|_{z_p = h_i} \quad i = 1, ..., N - 1; j = 1, ..., N. \quad (2.100)$$

A set of linear equations can be derived from the boundary conditions. The solution of this set of equations provides the parameters $A_{ij}$ and $B_{ij}$. These parameters are quite complex and are the fractions of exponential functions, which depend on $m$, $z_q$, $h_i$ and $k_i$. Hence it is very difficult to directly evaluate the Fourier integrals. However, by converting the denominators of $A_{ij}$’s and $B_{ij}$’s into power series, the integrals (2.96) can be evaluated. It appears that the Green’s function obtained by integrating (2.96) is similar to the one found by the method of images. The Green’s function obtained can be written as a one dimensional sum of terms:

$$g(z_p, z_q, r) = \sum_{i=0}^{\infty} \frac{s_i}{\sqrt{r^2 + (z_p + z_i)^2}} \quad (2.101)$$

In Equation (2.101) we use the following notation:

- $s_i$ - the image strength;
- $z_i$ - the position of the image (height) above the ground plane which can be expressed as $(x_i + \sigma_i z_q)$, with $\sigma_i = \pm 1$;

The singular term (free space term) and the first image about the ground plane form a pair with the same strength. Careful analysis of the series as given by (2.101)
2.6 Integration of the Green’s function

shows that the rest of the images can be collected into groups with the same absolute strength:

\[
\begin{align*}
\frac{s_i}{\sqrt{r^2 + (z_p - x_i + z_q)^2}} & \quad \frac{-s_i}{\sqrt{r^2 + (z_p + x_i - z_q)^2}}, \\
\frac{s_i}{\sqrt{r^2 + (z_p + x_i + z_q)^2}} & \quad \frac{-s_i}{\sqrt{r^2 + (z_p - x_i - z_q)^2}}
\end{align*}
\]

Equation (2.101) expresses the Green’s function formulation we are working with.

2.6 Integration of the Green’s function

After the discretization of the conductor surface into triangular elements, the integrals of the Green’s function and of its normal derivative must be calculated.

In this section we consider the integral of the Green’s function:

\[
G_{ij} = \int_{p \in S_p} \int_{q \in S_q} G(p, q) f_i(p) f_j(q) dq dp
\]

Since we know that the shape functions are constant and normalized, i.e. \( f_i(p) = \frac{1}{S_i} \) with \( S_i \) the area of the element where point \( p \) lies and by analogy \( f_j(q) = \frac{1}{S_j} \) with \( S_j \) the area of the element where \( q \) lies, we can simplify (2.103) to the form:

\[
G_{ij} = \frac{1}{S_i S_j} \int_{p \in S_p} \int_{q \in S_q} G(p, q) dq dp
\]

The most difficult problem, in computing the influence matrix \( G \) is the singularity resulting from the Green’s function, especially for the diagonal elements when the integration is performed twice over the same element. The usual way to handle this singularity is by finding a suitable substitution which allows to remove the singularity from the integrand. Another method to cope with singularities is to calculate the outer integrals numerically while the inner integrals are evaluated analytically. Analytical calculation of these integrals is not a simple matter. In [Wilton 84] and [Graglia 93] one can find the analytical integral formulas for the potential due to a uniform or linear source distribution.

Analytical evaluation of the integrals is done by using an appropriate Gauss’s integral theorem (the divergence theorem) to transform the integration over the planar element \( S \) into an integration over the boundary of the element \( \partial S \). Such a theorem is applicable when the integrand is continuously differentiable on the domain of integration.

When the point \( p \), which is the projection of the observation point \( p \) on the plane of the triangular element \( S \), falls inside the element \( S \) or on its contour \( \partial S \), this is not the case anymore. One must split the region \( S \) into the region \( S_i \), which is defined
as the intersection of $S$ and a small disk of radius $\varepsilon$ centered at $\rho$, and $(S - S_\varepsilon)$. With integrals over $S_\varepsilon$ or its boundary $\partial S_\varepsilon$, we have to be very careful. They can be evaluated by expressing them in terms of a local polar coordinate system with its origin centered at the point $\rho$. Such integrals involve the angular extent $\alpha(\rho)$ of the circular arc portion of $\partial S_\varepsilon$ lying within $S$. Therefore, we can distinguish the following four cases:

1. $\alpha(\rho) = 0$ if $\rho$ is outside $S$;
2. $\alpha(\rho) = 2\pi$ if $\rho$ is inside $S$;
3. $\alpha(\rho) = \pi$ if $\rho$ is on the edge of the contour $\partial S$ but not in the corner;
4. $\alpha(\rho) = \alpha$ if $\rho$ is a vertex of $S$, $\alpha$ is then the angle between the two edges of $\partial S$ meeting at the vertex ($0 < \alpha < \pi$).

The last three cases are illustrated in Figure 2.11(a–c), showing the angular extent.

![Figure 2.11. The angular extent as the circular arc portion of $\partial S_\varepsilon$ lying within $S$.](image)

The formula for analytical integration presented in [Wilton 84] has many advantages in terms of accuracy, conciseness, and convenience for numerical work.

Once the analytical integration is performed, the outer integration can be calculated by using e.g. an integration formula as given in [Stroud 71]. In a Gaussian quadrature integration formula a number of sample points in the triangle are chosen in which the inner integral is evaluated. The values of the inner integrals in these points are summed together with proper weights, see [Stroud 71], to provide reliable results. One may choose, e.g. between 3 point, 7 point or 16 point formulas which, by using an appropriate mapping, can be applied to any arbitrary triangular element. In general, the more points in the element, the better the result of the numerical integration. An increase of the number of sample points can be achieved by using a higher order formula which use more points. Alternatively one may use a lower order integration with less points, and then to apply these formulas for triangular sub-elements obtained by subdivision of the original triangular element as explained in [Zwillinger 92]. In Section 2.7.2 we present a practical implementation of the latter scheme.
2.7 Integration of the normal derivative of the Green’s function

If the integrals of the Green’s function do not contain any singularity, i.e. the integration is performed over different elements, both the inner and outer integrals can be computed by using numerical Gaussian quadrature.

Details of the integration technique which we have used, and discussion of the convergence, can be found in [Meijs 94]. Here, a trade-off is made between the exact but time consuming analytical integration and the quicker but less accurate numerical integration. The main diagonal elements of the $G$ matrix are evaluated analytically, while the off-diagonal elements are evaluated numerically. To improve the convergence of the integration for off-diagonal elements, in special cases, we conditionally switch to analytical integration.

2.7 Integration of the normal derivative of the Green’s function

In the previous section we have shown how the integration of the Green’s function can be performed. But in the boundary integral equation also the integral of the normal derivative of the Green’s function is involved. In this section we discuss the calculation of the integral of the normal derivative of the Green’s function.

2.7.1 Singularities

We have decided to use numerical integration for both inner and outer integration, since it straightforward to deal with this integral. However, we must take care of eventual singularities.

Let us start with constructing the integrand, i.e. the normal derivative of the Green’s function. We will work with the free space Green’s function:

$$G(p, q) = \frac{1}{4\pi k \sqrt{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2}}.$$  \hfill (2.105)

where $(x_q, y_q, z_q)$ are the coordinates of the source point $q$ and $(x_p, y_p, z_p)$ are the coordinates of the observation point $p$. The normal derivative of the Green’s function becomes:

$$\frac{\partial G}{\partial n_q}(p, q) = \nabla G(x_p, y_p, z_p|x_q, y_q, z_q) \cdot n_q,$$  \hfill (2.106)

with $n_q$ the normal vector to the face containing the source point $q$.

Writing $n_q = (n_{qx}, n_{qy}, n_{qz})$ we obtain:

$$\frac{\partial G}{\partial n_q}(p, q) = n_{qx} \frac{\partial}{\partial x_q} G(x_p, y_p, z_p|x_q, y_q, z_q) + n_{qy} \frac{\partial}{\partial y_q} G(x_p, y_p, z_p|x_q, y_q, z_q) + n_{qz} \frac{\partial}{\partial z_q} G(x_p, y_p, z_p|x_q, y_q, z_q).$$  \hfill (2.107)
with:

\[
\frac{\partial}{\partial x_q} G(p, q) = \frac{1}{4\pi k \left[ (x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2 \right]^{3/2}} (x_p - x_q)
\]

\[
\frac{\partial}{\partial y_q} G(p, q) = \frac{1}{4\pi k \left[ (x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2 \right]^{3/2}} (y_p - y_q)
\]

\[
\frac{\partial}{\partial z_q} G(p, q) = \frac{1}{4\pi k \left[ (x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2 \right]^{3/2}} (z_p - z_q)
\]

(2.108)
(2.109)
(2.110)

A singularity appears when the point \( p \) overlaps with the point \( q \). We distinguish three singular cases depending on the location of \( p \) and \( q \):

1. \( p \) lies inside the element;
2. \( p \) lies on the edge of an element;
3. \( p \) lies in the vertex of an element.

Let us study each of these cases. For the purpose of constructing the matrix \( G^{(n)} \) we have to calculate the following double integral:

\[
\frac{1}{4\pi k} \int_{p \in S_p} \int_{q \in S_q} \left[ \frac{n_{pq}(x_p - x_q)}{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2} + \frac{n_{p}\,(y_p - y_q)}{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2} + \frac{n_{q}\,(z_p - z_q)}{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2} \right] dp \, dq.
\]

(2.111)

We consider an arbitrary triangular face in a local coordinate system with origin in one of the nodes of the triangle lying in the \( xy \) plane, as shown in Figure 2.12. The normal vector to the triangular face in the local coordinate system is \( [0 \ 0 \ 1]^T \).

Hence the integral given by (2.111) reduces to:

\[
\frac{1}{4\pi k} \int_{p \in S_p} \int_{q \in S_q} \frac{\partial G(p, q)}{\partial n_q} \, dq \, dp = \frac{1}{4\pi k} \int_{p \in S_p} \int_{q \in S_q} \left[ \frac{(z_p - z_q)}{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2} \right] dq \, dp.
\]

(2.112)

The inner integral over \( S_q \) is given by:

\[
\frac{1}{4\pi k} \int_{q \in S_q} \frac{(z_p - z_q)}{r_{pq}^2 + (z_p - z_q)^2} \, dq.
\]

(2.113)
2.7 Integration of the normal derivative of the Green’s function

It is clear that for \( r_{pq} \neq 0 \) and \( z_p = z_q \) the integrand is equal zero. Thus the result of the double integration is zero as well. When \( r_{pq} = 0 \) the integrand becomes singular and special treatment of the integral is required. We take an arbitrary point \( q \) inside the triangular face surrounded by a small circular neighborhood \( S_\varepsilon \) with the radius \( \varepsilon \) centered at \( q \).

A coordinate transformation into a local polar coordinate system gives:

\[
x_q = r \cos \phi, \tag{2.114}
\]
\[
y_q = r \sin \phi, \tag{2.115}
\]
and the value of the Jacobian:

\[
J = \begin{vmatrix} \cos \phi & \sin \phi \\ -r \sin \phi & r \cos \phi \end{vmatrix} = r. \tag{2.116}
\]

Hence, the integral:

\[
\frac{1}{4\pi k} \int_{q \in S_\varepsilon} \frac{z_p - z_q}{\sqrt{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2}} \, dq \tag{2.117}
\]

in a polar coordinate system can be written as:

\[
\frac{1}{4\pi k} \int_0^\alpha \int_0^\varepsilon \frac{(z_p - z_q)r}{\sqrt{r^2 + (z_p - z_q)^2}} \, drd\phi = \frac{1}{4\pi k} \int_0^\alpha \int_0^\varepsilon \frac{(z_p - z_q)r}{\sqrt{r^2 + (z_p - z_q)^2}} \, dr \\
= \frac{1}{4\pi k} \alpha \left[ \frac{(z_p - z_q)}{|z_p - z_q|} - \frac{(z_p - z_q)}{\sqrt{\varepsilon^2 + (z_p - z_q)^2}} \right]. \tag{2.118}
\]
The last expression has the limit, for \( z_p \to z_q \), given by:

\[
\lim_{z_p \to z_q} \frac{\alpha}{4\pi k} \left( \frac{z_p - z_q}{|z_p - z_q|} \right) = \pm \frac{\alpha}{4\pi k} \quad (2.119)
\]

We take \( z_p > z_q \), hence the result of the inner integration is simply \( \alpha \), the angular extent mentioned in the last section, times the coefficient \( \frac{1}{4\pi k} \). Then:

- for \( p \) lying inside the triangle \( \alpha = 2\pi \);
- for \( p \) lying on the edge of the triangle \( \alpha = \pi \);
- for \( p \) lying in the vertex of the triangle \( \alpha = \beta \) with \( \beta \) the angle between the two edges of the triangle meeting at this vertex.

Only the first singularity will contribute to the outer integral. It can be shown that the corner and edge singularities do not influence the outer integration and their contribution is be zero.

### 2.7.2 Practical implementation

As mentioned before, we work with the Green’s function given in the form of an infinite series:

\[
g(z_p, z_q, r) = \sum_{i=1}^{\infty} \frac{s_i}{\sqrt{r^2 + (z_p + x_i + \sigma_i z_q)^2}}
\]

with \( r^2 = (x_p - x_q)^2 + (y_p - y_q)^2 \).

To obtain the normal derivative of this Green’s function, one must calculate the gradient of the Green’s function. Linearity of the gradient operation allows us to write:

\[
\nabla g(z_p, z_q, r) = \sum_{i=1}^{\infty} \nabla \frac{s_i}{\sqrt{r^2 + (z_p + x_i + \sigma_i z_q)^2}}
\]

If we denote by \( t_i(z_p, z_q, r) \) a single term from the series (2.120), then \( \nabla t_i(z_p, z_q, r) \) becomes:

\[
\nabla t_i(z_p, z_q, r) = \begin{bmatrix}
\frac{\partial t_i}{\partial x_p} \\
\frac{\partial t_i}{\partial y_p} \\
\frac{\partial t_i}{\partial x_q} \\
\frac{\partial t_i}{\partial y_q}
\end{bmatrix} = \frac{1}{[r^2 + (z_p + x_i + \sigma_i z_q)^2]^{3/2}} \begin{bmatrix}
s_i(x_p - x_q) \\
s_i(y_p - y_q) \\
-s_i(z_p + x_i + \sigma_i z_q)
\end{bmatrix}
\]

(2.122)
The normal derivative of the Green’s function for the normal vector \( n_q = [n_{qx}, n_{qy}, n_{qz}]^T \) is given by:

\[
\frac{\partial t_i}{\partial n_q} = n_q \cdot \nabla t_i(z_p, z_q, r) = \frac{g_i}{[r^2 + (z_p + x_i + \sigma_i z_q)^2]^{3/2}}
\]

\[
(n_{qx}(x_p - x_q) + n_{qy}(y_p - y_q) - n_{qz}\sigma_i(z_p + x_i + \sigma_i z_q))
\]

(2.123)

To calculate the integral:

\[
\int_{p \in S_p} \int_{q \in S_q} \frac{\partial t_i}{\partial n_q} dq dp
\]

we employ the Gaussian integration formula given in [Stroud 71].

Both outer and inner integration are treated with the same Gaussian formula. For a number of sample points in the triangles we evaluate the integrand and we add them up with proper weights \( W_i \)’s according to the formula:

\[
\int_{p \in S_p} \int_{q \in S_q} F(p, q) dq dp \approx \sum_{k=1}^{N} \sum_{j=1}^{N} [W_k W_j F(p_k, q_j)]
\]

(2.125)

with \( F(p_k, q_j) \) being the value of the integrand for the \( k^{th} \) point \( p_k \) in a triangle of area \( S_p \) and the \( j^{th} \) point \( q_j \) in a triangle of area \( S_q \). The \( W_i \)’s are the proper weights for the sample points.

In our case, \( F(p, q) = \frac{\partial t_i}{\partial n_q} \). Using the expressions (2.125) and (2.120) we can rewrite the integral \( \int_{p \in S_p} \int_{q \in S_q} \frac{\partial g}{\partial n_q} dq dp \) as:

\[
\int_{p \in S_p} \int_{q \in S_q} \frac{\partial g}{\partial n_q} dq dp = \sum_{i=0}^{\infty} \sum_{k=1}^{N} \sum_{j=1}^{N} W_k W_j F(p_k, q_j)
\]

(2.126)

The series over the index \( i \) is infinite and must be made finite by taking a certain number of terms. To determine what number of terms should be taken, we use an appropriate convergence criterion. Practical experiments with a numerical quadrature scheme show that the results obtained are insufficiently accurate. A method to improve the performance of the numerical integration is to sample the integrand at more nodes. However, the additional sampling needs to be performed only in problem areas. Thus we employ an adaptive integration which automatically increases the accuracy of a numerical approximation to the integral by increasing the number of sampling points. In our case we deal with a double integration in 3D space over triangular faces. For each term of the Green’s function we have to perform the numerical integration given by (2.125). Let us rewrite expression (2.125) as:

\[
\int_{p \in S_p} \int_{q \in S_q} F(p, q) dq dp \approx \sum_{k=1}^{N} \sum_{j=1}^{N} W_k W_j F(p_k, q_j)
\]

(2.127)
We say that the numerical approximation of the double integral of the term will be accurate if the numerical approximation of the inner integral is accurate. For a chosen point \( p_k \) on the face \( S_q \) we have developed an adaptive scheme to calculate an accurate approximation to \( \int_{q \in S_q} F(p_k, q) \, dq \).

The recursive integral approximation \( F_{rec}(p, S_q) \) is computed as follows:

1. For a given triangle \( S_q \) and a given point \( p_k \) compute – using a Gaussian formula – the approximate integral \( I_{\text{Unsplit}} \), given as:

\[
I_{\text{Unsplit}} = \int_{q \in S_q} F(p_k, q) \, dq \, dp \approx \sum_{j=1}^{N} W_j F(p_k, q_j)
\]  

(2.128)

2. Split the triangle \( S_q \) into four sub-triangles \( S_{q1}, S_{q2}, S_{q3}, S_{q4} \) by taking the midpoints of the sides of \( S_q \), and constructing \( S_{q1}, ..., S_{q4} \) following the scheme of Figure 2.13.

\[
S_q = S_{q1} + S_{q2} + S_{q3} + S_{q4}
\]

Figure 2.13. Decomposition of the triangular element into four sub-triangles by joining the midpoints of the sides of the original triangular element.

3. For each of the sub-triangles \( S_{q1}, ..., S_{q4} \) compute the appropriate integral (as under step 1) and sum these together to form \( I_{\text{Split}} \), given by:

\[
I_{\text{Split}} = \sum_{l=1}^{4} \int_{q \in S_{ql}} F(p_k, q) \, dq = \sum_{l=1}^{4} \sum_{j=1}^{N} W_j F(p_k, q_{lj})
\]  

(2.129)

4. Evaluate the local error \( \delta_e \) given by:

\[
\delta_e = \left| \frac{I_{\text{Unsplit}} - I_{\text{Split}}}{I_{\text{Split}}} \right|
\]  

(2.130)

(a) If the local error \( \delta_e \) is small enough return the (more accurate) \( I_{\text{Split}} \) as the result of the integral.
2.8 Conclusions

(b) Otherwise, if $\delta_i$ does not satisfy the convergence constraint, perform the recursive integral scheme, starting at step 1, for each of the sub-triangles $S_{q_1}, \ldots, S_{q_4}$, and sum these to form:

$$I_{\text{rec}} = \sum_{i=1}^{4} F_{\text{rec}}(p_i, S_{q_i})$$

return the value of $I_{\text{rec}}$ as the result of the integral.

This process is repeated until convergence of the approximation of the original integral is reached. We illustrate this procedure in Figure 2.14 and Figure 2.15.

![Tree representation of the recursive integration for a sample point $p_i$ and the triangle $S_q$.](image)

Analysis of the number of nodes in the tree, where one node represents a single evaluation of the integral, shows that complexity of the tree in terms of number of nodes is of order $O(4^L)$ with $L$ being the depth of the tree and assuming that the tree is full. In practical cases the tree will not be full, but still its complexity will exhibit exponential behavior.

2.8 Conclusions

In this chapter we have presented the theoretical background and mathematics of the boundary element method. We have shown how this method can be applied to the modeling problem in IC's in order to obtain reliable and accurate capacitive models. We have also discussed various aspects of the practical implementation of the BEM.
Figure 2.15. Recursive scheme for the inner integration. Stages: (a) refinement, (b) local refinement, (c) sub-local refinement, (d) local convergence reached, (e) refinement of the subsequent sub-element.
Bibliography


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Chapter 3

THE FINITE ELEMENT METHOD

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3.1 Introduction

The computation of the capacitance for the interconnections of VLSI circuits brings the interior problem of Laplace's equation with boundary conditions into play. To solve this interior problem, i.e. to find a potential distribution in a specified region, the finite element method [Sakkas 79], [Horowitz 83], [Silvester 83], [Cottrell 85], [Kazil 86], [Straker 86] is often used. In this method, the 3D interconnection domain is subdivided into a number of tetrahedral elements. Of course one may use different shapes of finite elements, but from point of view of geometrical generality the tetrahedral shapes are advisable. With such tetrahedral elements one may fill in the modeled body much better concerning the volume of the body and also its boundaries. In order to find a potential distribution in the domain, the minimization of a quadratic functional of the energy stored in the bulk region is used as
an alternative formulation for Laplace’s equation. According to this, the potentials in all nodes at the boundaries and in the inner part of the domain are determined in terms of the solution of the finite element equations. The number of equations equals the number of nodes. Moreover, the matrix of the set of these simultaneous equations is sparse, symmetric and positive definite. The solution of this set of linear algebraic equations gives certain potential values and is equivalent to modeling each tetrahedral finite element by a network in which every edge is a capacitance.

In the present chapter we consider Laplace’s equation in the domain $\Omega$:

$$\nabla_p[k(p)\nabla_p\Phi(p)] = 0$$  \hspace{1cm} (3.1)

with the Dirichlet boundary conditions, i.e. with given potential on the boundary $S$ of the domain $\Omega$.

To generate a finite element model we take the following steps:

1. discretization of the solution domain;
2. approximation of the potential;
3. formulation for the element;
4. assembly of the elements;
5. imposing the constraints;
6. solution of the set of algebraic equations;
7. computation of derived variables;
8. construction of the relevant capacitance model;

In the present chapter we will give a description of all the steps listed above.

### 3.2 Discretization

The first step that we consider in the development of a finite element model is the discretization of the solution domain $\Omega$. Typical finite elements in a 3D space are of the form of parallelepipeds or tetrahedrons, the latter being preferable from the point of view of geometric generality. Using a tetrahedral mesh we can obtain a much better discretization at the boundary of the 3D domain we model. It should be obvious that no matter which finite elements we use there is in general an inherent error in modeling of the shape of the solution domain $\Omega$. The effect of these errors can be shown to diminish when the size of the elements gets smaller.

A typical discretization using tetrahedral elements is displayed in Figure 3.1. We indicate in this figure nodes, elements and interelement boundaries.
3.3 Approximation of the potential

Let us consider the single tetrahedral finite element, shown in Figure 3.2, as the \( j \)th element in the finite elements mesh.

![Figure 3.1. Typical tetrahedral mesh.](image)

![Figure 3.2. The tetrahedral element in three-dimensional space.](image)
For such an element we have:

\((x_{ji}, y_{ji}, z_{ji}) = 1, 2, 3, 4\) - the coordinates of the four vertices of the \(j^{th}\) tetrahedron;

\(\phi_{j1}, \phi_{j2}, \phi_{j3}, \phi_{j4}\) - the potentials at the vertices of the \(j^{th}\) element;

\(\Delta_j\) - the volume of the \(j^{th}\) element;

\(k_j\) - the dielectric permittivity assigned to the \(j^{th}\) element, which is constant within the element.

We assume that the potential within a typical tetrahedral element is approximated by an affine linear expression:

\[
\Phi^{(j)}(x, y, z) = \alpha_1 + \alpha_2 x + \alpha_3 y + \alpha_4 z
\]

\[= \begin{bmatrix} 1 & x & y & z \end{bmatrix} \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \end{bmatrix}^T, \quad (3.2)
\]

in which the four constant coefficients \(\alpha_1, \alpha_2, \alpha_3, \alpha_4\) must be determined.

We obtain these coefficients from the four independent simultaneous equations requiring that \(\Phi^{(j)}\) reaches the nodal values at the vertices of the tetrahedron, namely:

\[
\begin{bmatrix}
\Phi(x_{j1}, y_{j1}, z_{j1}) \\
\Phi(x_{j2}, y_{j2}, z_{j2}) \\
\Phi(x_{j3}, y_{j3}, z_{j3}) \\
\Phi(x_{j4}, y_{j4}, z_{j4})
\end{bmatrix}
= \begin{bmatrix}
\phi_{j1} \\
\phi_{j2} \\
\phi_{j3} \\
\phi_{j4}
\end{bmatrix}
= \begin{bmatrix}
1 & x_{j1} & y_{j1} & z_{j1} \\
1 & x_{j2} & y_{j2} & z_{j2} \\
1 & x_{j3} & y_{j3} & z_{j3} \\
1 & x_{j4} & y_{j4} & z_{j4}
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4
\end{bmatrix}.
\]

From this, straightforward, we have:

\[
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4
\end{bmatrix}
= \begin{bmatrix}
1 & x_{j1} & y_{j1} & z_{j1} \\
1 & x_{j2} & y_{j2} & z_{j2} \\
1 & x_{j3} & y_{j3} & z_{j3} \\
1 & x_{j4} & y_{j4} & z_{j4}
\end{bmatrix}^{-1}
\begin{bmatrix}
\phi_{j1} \\
\phi_{j2} \\
\phi_{j3} \\
\phi_{j4}
\end{bmatrix}, \quad (3.3)
\]

or

\[
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4
\end{bmatrix}
= N^{-1}
\begin{bmatrix}
\phi_{j1} \\
\phi_{j2} \\
\phi_{j3} \\
\phi_{j4}
\end{bmatrix}, \quad (3.5)
\]

where

\[
N = \begin{bmatrix}
1 & x_{j1} & y_{j1} & z_{j1} \\
1 & x_{j2} & y_{j2} & z_{j2} \\
1 & x_{j3} & y_{j3} & z_{j3} \\
1 & x_{j4} & y_{j4} & z_{j4}
\end{bmatrix}
\]

(3.6)

is a Vandermonde matrix. It is known that for four vertices of a tetrahedron which are not coplanar, the determinant of the matrix \(N\) has non-zero value that guarantees the existence of the inverse \(N^{-1}\).
3.3 Approximation of the potential

Substituting Equation (3.4) into Equation (3.2) we obtain a new expression for the approximate potential within the \( j \)th element:

\[
\Phi^{(j)}(x, y, z) = \begin{bmatrix} 1 & x & y & z \end{bmatrix} N^{-1} \begin{bmatrix} \phi_{j1} \\ \phi_{j2} \\ \phi_{j3} \\ \phi_{j4} \end{bmatrix}.
\]  

(3.7)

Let us define four functions \( f_{ji}(x, y, z), i = 1, 2, 3, 4 \) such that:

\[
\Phi^{(j)}(x, y, z) = \begin{bmatrix} f_{j1}(x, y, z) \\ f_{j2}(x, y, z) \\ f_{j3}(x, y, z) \\ f_{j4}(x, y, z) \end{bmatrix}^T \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix}.
\]  

(3.8)

It follows from Equation (3.7) that:

\[
\begin{bmatrix} f_{j1}(x, y, z) \\ f_{j2}(x, y, z) \\ f_{j3}(x, y, z) \\ f_{j4}(x, y, z) \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_{j1} & x_{j2} & x_{j3} & x_{j4} \\ y_{j1} & y_{j2} & y_{j3} & y_{j4} \\ z_{j1} & z_{j2} & z_{j3} & z_{j4} \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix}.
\]  

(3.9)

The functions \( f_{ji}(x, y, z), i = 1, 2, 3, 4 \) are often called the local basis or shape functions and are basic interpolation functions. The function \( f_{ji}(x, y, z) \) has the property that it is 1 in the \( j \)th node of the \( j \)th element and 0 in the other nodes of the \( j \)th element, it varies linearly inside the element and it is zero outside the \( j \)th element.

In Figure 3.3 we present the linear local shape functions associated with the \( j \)th node of the \( j \)th finite element in the first three dimensions: 1D, 2D and 3D. The visualization of a shape function for 3D finite elements causes some problems since the value of a shape function is in the 'fourth' dimension. The analogy between 1D and 2D elements should clarify the construction in 3D. In Figure 3.4 we show four shape functions associated with the \( j \)th tetrahedral element.

The expression for the approximate potential within a single tetrahedral element \( j \) of the mesh can then be written as:

\[
\Phi^{(j)}(x, y, z) = \sum_{i=1}^{4} f_{ji}(x, y, z) \phi_{ji},
\]  

(3.10)

with \( f_{ji}(x, y, z), i = 1, 2, 3, 4 \) the set of four shape functions assigned to the element \( j \).

Let us define the parameter \( \Delta_j \):

\[
\Delta_j = \frac{1}{6} \det N = \frac{1}{6} \begin{vmatrix} 1 & x_{j1} & y_{j1} & z_{j1} \\ 1 & x_{j2} & y_{j2} & z_{j2} \\ 1 & x_{j3} & y_{j3} & z_{j3} \\ 1 & x_{j4} & y_{j4} & z_{j4} \end{vmatrix}.
\]  

(3.11)
Figure 3.3. Examples of shape functions for different elements in: (a) 1D, (b) 2D and (c) 3D (dashed lines are in a 4th dimension).

Figure 3.4. Elemental local shape functions.
3.3 Approximation of the potential

which is the volume of the \( j^{th} \) tetrahedron. To ensure that the value of \( \Delta_j \) is positive a certain numbering of the nodes in the tetrahedral element must be enforced, namely the numbering that proceeds 'counterclockwise' around the element, according to the 'right-hand rule'.

Let us consider a system of four non-coplanar points determining a tetrahedron, as depicted in Figure 3.5. The points \( p_1, p_2 \) and \( p_3 \) determine the plane in which vectors \( p_1\hat{p}_2 \) and \( p_1\hat{p}_3 \) are lying. The operation of the cross product \( p_1\hat{p}_2 \times p_1\hat{p}_3 \) produces the vector \( \vec{n} \) perpendicular to the plane containing points \( p_1, p_2 \) and \( p_3 \). If the point \( p_4 \) lies on the side of the plane, containing points \( p_1, p_2, p_3 \), to which the vector \( \vec{n} \) points, we say the node numbering proceeds 'counterclockwise' around the tetrahedron. We show examples of a good and bad numbering in Figure 3.6.

The local shape function associated with the \( k^{th} \) node in the \( j^{th} \) element can be

![](image)

Figure 3.5. Explanation of the right-hand rule principle.

![](image)

Figure 3.6. (a) The correct 'counterclockwise' numbering of nodes in an element. (b) The incorrect numbering of nodes.
written as:
\[ f_{jk}(x, y, z) = \frac{1}{6\Delta} (-1)^{k+1} \{ (x_{k2} y_{k3} - x_{k3} y_{k2}) z_{k1} 
+ (x_{k3} y_{k1} - x_{k1} y_{k3}) z_{k2} 
+ (x_{k1} y_{k2} - x_{k2} y_{k1}) z_{k3} 
+ [(y_{k2} - y_{k3}) z_{k1} + (y_{k3} - y_{k1}) z_{k2} + (y_{k1} - y_{k2}) z_{k3}] x 
+ [(x_{k3} - x_{k2}) z_{k1} + (x_{k1} - x_{k3}) z_{k2} + (x_{k2} - x_{k1}) z_{k3}] y 
+ [(x_{k2} - x_{k3}) y_{k1} + (x_{k3} - x_{k1}) y_{k2} 
+ (x_{k1} - x_{k2}) y_{k3}] z \}. \] (3.12)

where the indices \( \{k, k_1, k_2, k_3\} \) are a circular ordering of the nodes \( \{1, 2, 3, 4\} \) given by:
\[
k_1 = (k \mod 4) + 1
k_2 = (k + 1 \mod 4) + 1
k_3 = (k + 2 \mod 4) + 1,
\] (3.13)

for example, with \( k = 2 \), we obtain \( \{k, k_1, k_2, k_3\} = \{2, 3, 4, 1\} \).

We have shown how the potential can be approximated within a single tetrahedral element. Let us generalize this approximation for the entire domain decomposed into a number \( M \) of tetrahedral finite elements. We assume that the system of \( M \) tetrahedrons forms a 3D mesh with, say, \( N \) nodes.

An approximate potential in the domain can then be expressed as:
\[
\tilde{\phi}(x, y, z) = \sum_{j=1}^{M} \sum_{i=1}^{4} f_{ji}(x, y, z) \phi_{ji},
\] (3.14)

where the \( f_{ji} \)'s are the local shape functions defined before. The formula (3.14) approaches the problem of approximating the potential from the point of view of \( M \) finite elements. We can reformulate expression (3.14) so that it views the approximation problem from the point of \( N \) nodes in a finite element mesh. It is easy to see that several indices \( j_i \) will correspond to the same point in the mesh. The same node may belong to different finite elements and it may have a different local numbering within each of the elements. Introducing a new numbering which uses an index \( k = 1, \ldots, N \), we can rewrite Equation (3.14) as:
\[
\tilde{\phi}(x, y, z) = \sum_{k=1}^{N} f_k(x, y, z) \phi_k,
\] (3.15)

where the functions \( f_k(x, y, z)_{k=1...N} \) are new shape functions which are called the conjoint shape functions. It is clear that a given conjoint shape function assigned to the \( k^{th} \) node can be considered to be composed of the sum of all the local shape functions coming from different finite elements assigned to the same node \( k \). In
3.3 Approximation of the potential

other words \( f_k(x_i, y_i, z_i) \) has a value 1 at the \( i^{th} \) node and it is 0 at all the other
nodes. Thus using Equation (3.15) we have:

\[
\Phi(x_i, y_i, z_i) = \sum_{k=1}^{N} f_k(x_i, y_i, z_i) \phi_k = \phi_i. 
\] (3.16)

We can say that the conjoint shape functions have local support, they have nonzero
values only in a small neighborhood of the node, which consists of only those ele­
ments which touch the node in consideration.

Again to clarify how the conjoint functions are constructed, we show in Figure 3.7
the analogy between 1D, 2D and 3D conjoint shape functions.

We expect that the finite element method will provide values for the approximate
potential \( \Phi(x, y, z) \) such that:

\[
\Phi(x, y, z) \approx \Phi(x, y, z). 
\] (3.17)
Figure 3.7. Changing of the basis from the local shape functions to the conjoint shape functions in: (a) 1D, (b) 2D and (c) 3D (dashed lines are in a 4th dimension).
3.4 Element formulation

These are two ways to develop the formulation of the FEM model:

1. the classical Galerkin method;

2. the equivalent minimization of energy (special case of minimal action principle) of the system.

In this section we present briefly the classical Galerkin approach while in the following section we will go into detail on the alternative method of minimization of energy.

3.4.1 The classical Galerkin method

Let us consider the Laplace’s equation:

\[ \nabla [k(x, y, z) \nabla \Phi(x, y, z)] = 0, \quad (3.18) \]

in the domain \( \Omega \), with Dirichlet boundary conditions on the boundary \( S \) of the considered domain.

Since \( \Phi(x, y, z) \) is not the exact solution, substitution of the approximate solution \( \tilde{\Phi}(x, y, z) \) into the governing equation produces a residual error \( R(x, y, z) \). Keeping in mind that \( \Phi \) and \( k \) are functions of \((x, y, z)\), we can write the error \( R(x, y, z) \) as:

\[ \frac{\partial}{\partial x} \left[ k \frac{\partial \tilde{\Phi}}{\partial x} \right] + \frac{\partial}{\partial y} \left[ k \frac{\partial \tilde{\Phi}}{\partial y} \right] + \frac{\partial}{\partial z} \left[ k \frac{\partial \tilde{\Phi}}{\partial z} \right] = R(x, y, z). \quad (3.19) \]

We assume that the approximate solution has the form given by Equation (3.16). Splitting the node potentials into the \( N \) internal potentials and \( M \) boundary potentials (3.16) can be written in the following form:

\[ \tilde{\Phi}(x, y, z) = \sum_{j=1}^{N+M} f_j(x, y, z) \phi_j \]

\[ = \sum_{i=1}^{N} f_i(x, y, z) \phi_i + \sum_{k=N+1}^{N+M} f_k(x, y, z) \phi_k, \quad (3.20) \]

here \( \phi_k \)'s are the node potentials on the boundary \( S \) and \( \phi_i \)'s are the unknown node potentials inside the domain.

The weighted residual method, the principles of this method we have explained in Section 2.3.5, requires that the weighted integral over the discretized domain \( \Omega \) of the error function \( R(x, y, z) \), with the weighting function \( w_i(x, y, z) \), will be zero, that is:

\[ \int_{\Omega} R(x, y, z) w_i(x, y, z) \, dx \, dy \, dz = 0 \quad \text{for} \quad i = 1, 2, \ldots, N \quad (3.21) \]
or

\[
\int_{\Omega} \left\{ \frac{\partial}{\partial x} [k \frac{\partial \Phi}{\partial x}] + \frac{\partial}{\partial y} [k \frac{\partial \Phi}{\partial y}] + \frac{\partial}{\partial z} [k \frac{\partial \Phi}{\partial z}] \right\} w_i(x, y, z) \, dx \, dy \, dz = 0
\]

for \( i = 1, \ldots, N. \) \hspace{1cm} (3.22)

The Galerkin method, in principle, requires the set of weighting functions to be equivalent to the set of shape functions used to approximate the exact solution. For \( w_i(x, y, z) = f_i(x, y, z) \) Equations (3.22) are called the Galerkin equations. We need to determine \( N \) parameters in an approximate solution (the unknown inside node potentials). Thus we choose the shape functions associated with the inside nodes as the weighting functions. The important property of this choice, which we need later, is that these shape functions vanish on the boundary \( S \). To calculate the integral in Equation (3.22) we use the integration by parts. First, using the following relation (we don’t write arguments of functions they remain the same as before):

\[
f_i \frac{\partial}{\partial x} [k \frac{\partial \Phi}{\partial x}] = \frac{\partial}{\partial x} [f_i k \frac{\partial \Phi}{\partial x}] - k \frac{\partial f_i}{\partial x} \frac{\partial \Phi}{\partial x},
\]

which holds for \( y \) and \( z \) as well, we express Equation (3.22) as:

\[
\int_{\Omega} \left\{ \frac{\partial}{\partial x} [f_i k \frac{\partial \Phi}{\partial x}] + \frac{\partial}{\partial y} [f_i k \frac{\partial \Phi}{\partial y}] + \frac{\partial}{\partial z} [f_i k \frac{\partial \Phi}{\partial z}] \right\} \, dx \, dy \, dz

- \int_{\Omega} k [\frac{\partial f_i}{\partial x} \frac{\partial \Phi}{\partial x} + \frac{\partial f_i}{\partial y} \frac{\partial \Phi}{\partial y} + \frac{\partial f_i}{\partial z} \frac{\partial \Phi}{\partial z}] \, dx \, dy \, dz = 0
\]

for \( i = 1, \ldots, N. \) \hspace{1cm} (3.24)

The divergence theorem states that:

\[
\int_{\Omega} \frac{\partial F(x, y, z)}{\partial x} \, dx \, dy \, dz = \int_{S} n_x F(x, y, z) \, dx \, dy \, dz,
\]

where \( n_x \) is the component of the unit outward normal vector \( n \) around the bounding surface \( S \). Similar expressions can be derived for \( y \) and \( z \).

Applying the divergence theorem to the first term in Equation (3.24), the Galerkin equations can be written as:

\[
\int_{S} [n_x \frac{\partial \Phi}{\partial x} + n_y \frac{\partial \Phi}{\partial y} + n_z \frac{\partial \Phi}{\partial z}] f_i \, dS

- \int_{\Omega} k [\frac{\partial f_i}{\partial x} \frac{\partial \Phi}{\partial x} + \frac{\partial f_i}{\partial y} \frac{\partial \Phi}{\partial y} + \frac{\partial f_i}{\partial z} \frac{\partial \Phi}{\partial z}] \, dx \, dy \, dz = 0
\]

for \( i = 1, \ldots, N. \) \hspace{1cm} (3.26)

Using the property:

\[
n_x \frac{\partial \Phi}{\partial x} + n_y \frac{\partial \Phi}{\partial y} + n_z \frac{\partial \Phi}{\partial z} = \frac{\partial \Phi}{\partial n},
\]

(3.27)
we rewrite Equation (3.26) as:

\[
\int_S \frac{\partial \Phi}{\partial n} f_i \, dx \, dy \, dz - \int_{\Omega} k \left[ \frac{\partial f_i}{\partial x} \frac{\partial \Phi}{\partial x} + \frac{\partial f_i}{\partial y} \frac{\partial \Phi}{\partial y} + \frac{\partial f_i}{\partial z} \frac{\partial \Phi}{\partial z} \right] \, dx \, dy \, dz = 0
\]

for \( i = 1, \ldots, N \). (3.28)

The next step in the formulation consists of simplifying the boundary terms with the aid of the specified boundary conditions. Since \( f_i \)'s chosen for the weighting functions vanish on the boundary \( S \), the first integral in Equation (3.28) cancels out. Hence (3.28) becomes:

\[
\int_{\Omega} k \left[ \frac{\partial f_i}{\partial x} \frac{\partial \Phi}{\partial x} + \frac{\partial f_i}{\partial y} \frac{\partial \Phi}{\partial y} + \frac{\partial f_i}{\partial z} \frac{\partial \Phi}{\partial z} \right] \, dx \, dy \, dz = 0
\]

for \( i = 1, \ldots, N \). (3.29)

Substituting Equation (3.20) into (3.29) we arrive at:

\[
\int_{\Omega} k \left[ \frac{\partial f_i}{\partial x} \left( \sum_{j=1}^{N+M} \phi_j \frac{\partial f_j}{\partial x} \right) + \frac{\partial f_i}{\partial y} \left( \sum_{j=1}^{N+M} \phi_j \frac{\partial f_j}{\partial y} \right) + \frac{\partial f_i}{\partial z} \left( \sum_{j=1}^{N+M} \phi_j \frac{\partial f_j}{\partial z} \right) \right] \, dx \, dy \, dz = 0
\]

for \( i = 1, \ldots, N \), (3.30)

or in matrix notation:

\[
H\Phi = 0,
\]

with the entry \( h_{ij} \), for \( i = 1, \ldots, N \) and \( j = 1, \ldots, N + M \), of the \( H \) matrix given by:

\[
h_{ij} = \int_{\Omega} k \left[ \frac{\partial f_i}{\partial x} \frac{\partial f_j}{\partial x} + \frac{\partial f_i}{\partial y} \frac{\partial f_j}{\partial y} + \frac{\partial f_i}{\partial z} \frac{\partial f_j}{\partial z} \right] \, dx \, dy \, dz.
\]

(3.32)

Splitting the vector of node potentials \( \Phi \) into the vector of boundary potentials \( \phi_b \) and internal potentials \( \phi_i \), we can rewrite Equation (3.31) as:

\[
\begin{bmatrix}
H_{ib} & H_{ii}
\end{bmatrix}
\begin{bmatrix}
\phi_i \\
\phi_b
\end{bmatrix} = 0.
\]

(3.33)

Solving Equation (3.33) and assuming that the matrix \( H_{ii} \) is invertible we obtain the unknown \( N \) internal node potentials, given by:

\[
\phi_i = -H_{ii}^{-1} H_{ib} \phi_b,
\]

(3.34)

and the resulting distribution of the potential becomes:

\[
\Phi = \begin{bmatrix}
\phi_b \\
-H_{ii}^{-1} H_{ib} \phi_b
\end{bmatrix}.
\]

(3.35)
3.4.2 Energy approach

In this section we present the energy approach to solve the potential distribution inside the domain \( \Omega \). As we shall see later on in Section 3.6 this approach produces identical results to the classical Galerkin method presented in the previous section, since it uses the property that the error of the function to be approximated must be orthogonal to all possible approximating functions.

The minimization of energy approach is much better for visualization of the assembly of elements and it allows a much easier explanation of the model construction.

First, let us give some foundations of the energy method. Let us consider the interior problem of the Laplace equation in the domain \( \Omega \), with the Dirichlet boundary conditions on the boundary \( S \) of the domain. Our goal is to find the distribution of the potential inside the domain \( \Omega \).

It is an obvious principle that all physical systems tend to the state in which they keep a minimal energy. Informally we can say that “nature is lazy” or that “nature searches for the solution that minimizes energy”. Therefore to get an approximate solution of the Laplace’s equation, which is the governing equation in the domain under consideration, it remains to minimize the energy stored in the domain. The energy of the system is expressed by a quadratic functional (the integral). The unconstrained minimum of the energy functional trivially equals zero and gives zero potential everywhere. This trivial solution does not correspond to a real physical situation. To obtain a solution which is the closest to an exact solution, we account for the boundary conditions, i.e. the potential at the boundary must be specified.

Let \( \Omega \) be a 3D interconnection domain surrounded by a sufficiently smooth boundary \( S \). For a point \( p = (x, y, z) \), in \( \Omega \) or on \( S \), we define the potentials \( \Phi(p) \) and \( \Psi(p) \) and the dielectric permittivity \( k(p) \), all sufficiently smooth functions. Moreover, let \( n \) be the outgoing unit normal on \( S \) and \( \nabla_p \) the gradient at the point \( p = \nabla_p = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right] \).

We can formulate the following theorem about the solution of the potential.

**Theorem 1** If \( \Phi(p) \) is the solution of the Laplace’s equation:

\[
\nabla_p [k(p)\nabla_p \Phi(p)] = 0,
\]

which satisfies a given boundary condition on \( S \), then it minimizes the energy functional:

\[
E(\Phi(p)) = \int_\Omega k(p)\|\nabla_p \Phi(p)\|^2 \, dp
\]

over all functions \( \Phi(p) \) for which the gradient exists and for which the integral is well-defined.
3.4 Element formulation

**Proof**

We claim that the function \( \Phi(p) \) that satisfies Equation (3.36) with the given boundary conditions is exactly the potential that minimizes the energy functional (3.37). Suppose that \( \Psi(p) \) is a perturbation function such that \( \Psi(p) = 0 \) on \( S \) and \( \Psi(p) \) is sufficiently smooth. Then:

\[
\mathcal{E}(\Phi(p) + \Psi(p)) = \frac{1}{2} \int_\Omega k(p) \| \nabla_p (\Phi(p) + \Psi(p)) \|^2 \, dp \\
= \frac{1}{2} \int_\Omega k(p) \| \nabla_p \Phi(p) \|^2 \, dp + \frac{1}{2} \int_\Omega k(p) \| \nabla_p \Psi(p) \|^2 \, dp \\
+ \int_\Omega k(p)(\nabla_p \Psi(p))(\nabla_p \Phi(p)) \, dp. \tag{3.38}
\]

By using:

- Green’s theorem:
  \[
  \int_\Omega \Psi(p) \nabla_p [k(p) \nabla_p \Phi(p)] \, dp = \int_S \Psi(p) k(p) \frac{\partial \Phi(p)}{\partial n} \, dp \\
  - \int_\Omega \nabla_p \Psi(p) [k(p) \nabla_p \Phi(p)] \, dp; \tag{3.39}
  \]

- the boundary condition for \( \Psi(p) \) on the boundary \( S \):
  \[
  \Psi(p) = 0 \text{ on } S; \tag{3.40}
  \]

- the fact that \( \Phi \) satisfies Equation (3.36),

the last term in Equation (3.38) evaluates to zero as:

\[
\int_\Omega k(p)(\nabla_p \Phi(p))(\nabla_p \Psi(p)) \, dp = \int_S k(p) \Psi(p) \frac{\partial \Phi(p)}{\partial n} \, dp \\
- \int_\Omega \Psi(p) \nabla_p [k(p) \nabla_p \Phi(p)] \, dp \\
= 0. \tag{3.41}
\]

Hence:

\[
\mathcal{E}(\Phi(p) + \Psi(p)) = \mathcal{E}(\Phi(p)) + \mathcal{E}(\Psi(p)), \tag{3.42}
\]

which is clearly minimal for \( \Psi(p) = 0 \), since \( \mathcal{E} \) is a strictly positive functional.

The theorem presented above is fundamental for the FEM. It allows us to use the minimization of the quadratic functional of the energy stored in the bulk region as an alternative formulation for the Laplace’s equation.
3.4.3 Element analysis

We use the same notation as in Section 3.3. The energy associated with a single element \( j \) is defined by:

\[
\mathcal{E}^{(j)} = \frac{1}{2} \int_{j} \kappa_j \| \nabla_p \Phi^{(j)}(p) \|^2 \, dp. \tag{3.43}
\]

Since the region of integration is the element itself, the gradient of the potential within the element given by Equation (3.10) may be determined by the formula:

\[
\nabla_p \Phi^{(j)}(p) = \sum_{i=1}^{4} \phi_{ji} \nabla_p f_{ji}(p). \tag{3.44}
\]

Referring to Equation (3.12) and (3.13) the gradients of the local shape functions associated with each node of the \( j \)th finite element are given by:

\[
\nabla_p f_{jk}(p)|_{p=(x,y,z)} = \frac{1}{6\Delta_j} (-1)^{k+1} \left\{ (y_{k2} - y_{k3}) z_{k1} + (y_{k3} - y_{k1}) z_{k2} + (y_{k1} - y_{k3}) z_{k3} \right\} e_x
\]

\[
+ \left\{ (x_{k1} - x_{k3}) z_{k1} + (x_{k2} - x_{k3}) z_{k2} \right\} e_y
\]

\[
+ \left\{ (x_{k2} - x_{k1}) y_{k1} + (x_{k1} - x_{k3}) y_{k2} \right\} e_z
\]

where \( e_x, e_y \) and \( e_z \) are the unit vectors in the \( x, y \) and \( z \) direction, respectively.

The energy stored in the \( j \)th element becomes:

\[
\mathcal{E}^{(j)} = \frac{1}{2} \int_{j} \kappa_j \| \nabla_p \Phi^{(j)}(p) \|^2 \, dp
\]

\[
= \frac{1}{2} \int_{j} \kappa_j \nabla_p \Phi^{(j)}(p) \nabla_p \Phi^{(j)}(p) \, dp
\]

\[
= \frac{1}{2} \int_{j} \kappa_j \sum_{i=1}^{4} \phi_{ji} \nabla_p f_{ji}(p) \nabla_p f_{ji}(p) \, dp
\]

\[
= \frac{1}{2} \sum_{i=1}^{4} \phi_{ji} \phi_{ji} \int_{j} \kappa_j \nabla_p f_{ji}(p) \nabla_p f_{ji}(p) \, dp
\]

\[
= \frac{1}{2} \sum_{i=1}^{4} \sum_{l=1}^{4} \phi_{ji} \phi_{jl} \int_{j} \kappa_j \nabla_p f_{ji}(p) \nabla_p f_{jl}(p) \, dp
\]

\[
= \frac{1}{2} \sum_{i=1}^{4} \sum_{l=1}^{4} \phi_{ji} h^{(j)}_{il} \phi_{jl}, \tag{3.45}
\]

with:

\[
h^{(j)}_{il} = \kappa_j \int_{j} \nabla_p f_{ji}(p) \nabla_p f_{jl}(p) \, dp. \tag{3.46}
\]
Let $\Phi^{(j)}$ be the column vector of the node potentials $\Phi^{(j)} = [\phi_{j1} \phi_{j2} \phi_{j3} \phi_{j4}]^T$, and $H^{(j)}$ the coefficients matrix such that:

$$H^{(j)} = \begin{bmatrix} h_{11}^{(j)} & h_{12}^{(j)} & h_{13}^{(j)} & h_{14}^{(j)} \\ h_{21}^{(j)} & h_{22}^{(j)} & h_{23}^{(j)} & h_{24}^{(j)} \\ h_{31}^{(j)} & h_{32}^{(j)} & h_{33}^{(j)} & h_{34}^{(j)} \\ h_{41}^{(j)} & h_{42}^{(j)} & h_{43}^{(j)} & h_{44}^{(j)} \end{bmatrix}.$$ (3.47)

$H^{(j)}$ is symmetric since $h_{ij}^{(j)} = h_{ji}^{(j)}$. The entries $h_{ij}^{(j)}$ are easy to compute. For instance, for $i = 1$ and $l = 2$, substitution of $\nabla_p f_{j1}(p)$ and $\nabla_p f_{j2}(p)$ into Equation (3.46) yields:

$$h_{12}^{(j)} = \frac{k_j}{36 \Delta_j} \left\{ [(y_{j3} - y_{j1})z_{j2} + (y_{j4} - y_{j2})z_{j3} + (y_{j2} - y_{j3})z_{j1}] \\
[(y_{j4} - y_{j3})z_{j1} + (y_{j1} - y_{j4})z_{j3} + (y_{j3} - y_{j1})z_{j4}] \\
+(x_{j4} - x_{j3})z_{j2} + (x_{j2} - x_{j4})z_{j3} + (x_{j3} - x_{j2})z_{j1}] \\
[(x_{j3} - x_{j4})z_{j1} + (x_{j1} - x_{j3})z_{j3} + (x_{j1} - x_{j3})z_{j1}] \\
+ [(x_{j3} - x_{j1})y_{j2} + (x_{j4} - x_{j2})y_{j3} + (x_{j2} - x_{j3})y_{j4}] \\
[(x_{j4} - x_{j3})y_{j1} + (x_{j1} - x_{j4})y_{j3} + (x_{j3} - x_{j1})y_{j4}] \right\}. \quad (3.48)$$

### 3.5 Element assembly

The total energy associated with an assembly of all elements, say $N$, is simply the sum of energies of all individual elements.

Let us define a column vector $\Phi_d$, which consists of all the node potentials of the individual elements:

$$\Phi_d^T = [\phi_{11} \phi_{12} \phi_{13} \phi_{14} \phi_{21} \phi_{22} \ldots \phi_{N3} \phi_{N4}], \quad (3.49)$$

and a coefficient matrix $H_d$ being a block-diagonal matrix:

$$H_d = \begin{bmatrix} H^{(1)} & & & 0 \\ & H^{(2)} & & \\ & & \ddots & \\ 0 & \ldots & & H^{(N)} \end{bmatrix}, \quad (3.50)$$

with $H^{(j)}$ being the $4 \times 4$ matrix associated with the $j^{th}$ element as defined in the previous section. The index "\(d\)" used in this section means "disjoint" and reminds us that we consider a disjoint system of independent elements with independent numbering of nodes in each tetrahedron.
The energy of the entire system then becomes:

\[
\mathcal{E}_t = \sum_{j=1}^{N} \mathcal{E}^{(j)} = \sum_{j=1}^{N} \frac{1}{2} (\Phi^{(j)})^T H^{(j)} \Phi^{(j)} = \frac{1}{2} \sum_{j=1}^{N} (\Phi^{(j)})^T H^{(j)} \Phi^{(j)} = \frac{1}{2} \Phi_d^T H_d \Phi_d.
\]  

(3.51)

In the connected assembly of elements, the potential values are physically required to be continuous across interelement boundaries. For the tetrahedral elements with a linear approximation of the potential within the element, this will be the case if the potentials at corresponding nodes are identical. This equality constraint at the nodes may be expressed in a matrix form, as a rectangular incidence matrix \( S \) which relates the disjoint potentials \( \Phi_d \) to the conjoint potentials, denoted by \( \Phi_c \):

\[
\Phi_d = S \Phi_c.
\]

(3.52)

The index "c" used here means "conjoint" and reminds us that it is a system of conjoint elements which is under consideration here.

In Figure 3.8 we show a system of three tetrahedrons with disjoint numbering of the nodes and conjoint numbering of nodes.

![Figure 3.8](image-url)  

**Figure 3.8.** Decomposition of the region of interest into tetrahedral elements. (a) Disjoint tetrahedral finite elements. (b) Conjoint tetrahedral finite elements.

We define the incidence matrix \( S \) as follows:

\[
S_{ij} = \begin{cases} 
1 & \text{if } i^{th} \text{ node in disjoint numbering is equivalent to } j^{th} \text{ node in conjoint numbering} \\
0 & \text{otherwise}
\end{cases}
\]

(3.53)
Substituting Equation (3.52) into (3.51), we obtain:

\[ \mathbf{E}_t = \frac{1}{2} \Phi_c^T S^T H_d S \Phi_c = \frac{1}{2} \Phi_c^T H \Phi_c, \]  

(3.54)

with

\[ H = S^T H_d S \]  

(3.55)

representing the assembled coefficient matrix of the “connected” problem.

To illustrate the structure of the matrices \( S \) and \( H \), we consider the case of three tetrahedrons shown in Figure 3.8. Since the four potential values are associated with each tetrahedron, all possible states of the three elements can be described by a column vector containing all twelve node potentials:

\[ \Phi_d = \begin{bmatrix} \phi_{11} & \phi_{12} & \phi_{13} & \ldots & \phi_{34} \end{bmatrix}^T. \]  

(3.56)

The matrix \( S \) relates the potentials at the twelve nodes to the potentials at the six conjoint nodes, and takes the form:

\[
S^T = \begin{bmatrix}
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
\]  

(3.57)

We substitute Equation (3.57) into (3.55) and obtain the assembled coefficient matrix of the connected problem as:

\[
H = \begin{bmatrix}
(h_{11}^{(1)} + h_{11}^{(2)}) & (h_{11}^{(1)} + h_{11}^{(2)}) & (h_{11}^{(1)} + h_{11}^{(2)}) \\
(h_{14}^{(1)} + h_{33}^{(1)} + h_{11}^{(3)}) & (h_{12}^{(1)} + h_{12}^{(2)} + h_{13}^{(3)}) & (h_{22}^{(1)} + h_{22}^{(2)} + h_{33}^{(3)}) \\
(h_{14}^{(1)} + h_{33}^{(1)} + h_{11}^{(3)}) & (h_{12}^{(1)} + h_{12}^{(2)} + h_{13}^{(3)}) & (h_{22}^{(1)} + h_{22}^{(2)} + h_{33}^{(3)}) \\
(h_{13}^{(1)} + h_{33}^{(3)}) & (h_{12}^{(1)} + h_{12}^{(2)}) & (h_{22}^{(1)} + h_{22}^{(2)}) \\
(h_{13}^{(1)} + h_{13}^{(3)}) & (h_{12}^{(1)} + h_{12}^{(2)}) & (h_{22}^{(1)} + h_{22}^{(2)}) \\
0 & 0 & 0
\end{bmatrix}.
\]  

(3.58)

The incidence matrix influences not only the formulation of the energy of the system, but also changes the shape functions from the local type to the conjoint type. Let \( F \) be a row-vector containing all local shape functions on the disjoint level:

\[
F = \begin{bmatrix} f_{11}(p) & f_{12}(p) & \ldots & f_{N3} & f_{N4} \end{bmatrix}.
\]  

(3.59)
and \( \Phi \) a vector containing all node potentials, say \( M \), in the conjoint system:

\[
\Phi = \Phi_c = \begin{bmatrix} \phi_1 & \phi_2 & \ldots & \phi_M \end{bmatrix}^T.
\]  

The approximate potential (in the domain), obtained by imposing the continuity condition in nodes, is given by:

\[
\Phi = FS\Phi_c
\]

where the product \([FS]\) is a row-vector such that every \( i^{th} \) component \([FS]_i\) is a new conjoint shape function associated with the \( i^{th} \) node (in the conjoint level numbering).

### 3.6 Solution of the potential

Let us assume that the node numbering in the connected model is such that all boundary nodes (denoted by the subscript “b”) are numbered first, all internal nodes (denoted by the subscript “i”) last.

Let us split the vector of potentials \( \Phi \), defined by Equation (3.60), into the vector of boundary potentials \( \Phi_b \) and the vector of internal potentials \( \Phi_i \):

\[
\Phi = \begin{bmatrix} \phi_b^T & \phi_i^T \end{bmatrix}^T,
\]

then the coefficient matrix \( H \) can be partitioned into:

\[
H = \begin{bmatrix} H_{bb} & H_{bi} \\ H_{ib} & H_{ii} \end{bmatrix}.
\]

Since \( H \) is symmetrical we have:

\[
H_{bi} = H_{ib}^T.
\]

The “discretized” energy of the entire system is then given by:

\[
E_t = \frac{1}{2} \begin{bmatrix} \phi_b^T & \phi_i^T \end{bmatrix} \begin{bmatrix} H_{bb} & H_{bi} \\ H_{ib} & H_{ii} \end{bmatrix} \begin{bmatrix} \phi_b \\ \phi_i \end{bmatrix}.
\]

To find the potential distribution in the domain we model, we have to find the vector \( \phi_i \) only, since the node potentials \( \phi_b \) on the boundary are known.

As has been mentioned, in order to determine the \( \phi_i \)'s we have to minimize the energy \( E_t \) given by Equation (3.65) over the \( \phi_i \)'s while keeping the \( \phi_b \)'s fixed. This can be done either in a straightforward way, or by use of an other minimization technique like, for example, the Lagrange multipliers method.
3.6 Solution of the potential

In the direct minimization, we calculate the derivative of the energy $\mathcal{E}_t$ over $\phi_i$'s and require that this derivative is zero. This procedure yields the matrix equation which, in partitioned form, can be written as:

\[
\begin{bmatrix}
H_{ib} & H_{ii}
\end{bmatrix}
\begin{bmatrix}
\phi_b \\
\phi_i
\end{bmatrix} = 0.
\] (3.66)

That is:

\[H_{ib}\phi_b + H_{ii}\phi_i = 0,\] (3.67)

or

\[\phi_i = -H^{-1}_{ii}H_{ib}\phi_b.\] (3.68)

A formal solution to the problem is therefore given by:

\[\Phi = \begin{bmatrix}
\phi_b \\
-H^{-1}_{ii}H_{ib}\phi_b
\end{bmatrix}.\] (3.69)

This is exactly the same result as was given by Equation (3.35) but obtained by the principle of minimal energy.

We will present the Lagrange multipliers method as well, which will prove useful later on for the model construction of the equivalent electrical circuit.

The adapted minimization procedure based on the Lagrange multipliers method consists of the following steps:

1. Derivation of the quadratic energy functional - subject to constrain;
   Referring to the previous sections and Equation (3.65) we write our subject to constrain as:
   \[\mathcal{E} = \frac{1}{2}\phi_b^T H_{bb}\phi_b + \frac{1}{2}\phi_i^T H_{ii}\phi_i + \phi_b^T H_{bi}\phi_i.\] (3.70)

2. Definition of the boundary conditions - constraints;
   We impose Dirichlet boundary conditions on the boundary of the considered domain, according to which the potential in the nodes at the boundary is known. This means that $\phi_b$ is fixed:
   \[\phi_b = \phi_{\text{fixed}}.\] (3.71)

3. Formulation of the object to minimize;
   To derive the object to minimize, let us first introduce the vector of Lagrange coefficients $\lambda$, of the same dimensions as $\phi_b$.
   Our object to minimize becomes:
   \[\mathcal{E} = \frac{1}{2}\phi_b^T H_{bb}\phi_b + \frac{1}{2}\phi_i^T H_{ii}\phi_i + \phi_b^T H_{bi}\phi_i + \lambda^T (\phi_b - \phi_{\text{fixed}}).\] (3.72)
4. Setting up the algebraic equations;

In order to construct the set of equations to solve, the partial derivatives of the object to minimize over \( \phi_b \)'s and \( \phi_i \)'s must be set to zero. The partial derivatives over \( \phi_b \)'s and \( \phi_i \)'s are respectively:

\[
\frac{\partial E_m}{\partial \phi_b} = H_{bb} \phi_b + H_{bi} \phi_i + \lambda, \tag{3.73}
\]

\[
\frac{\partial E_m}{\partial \phi_i} = H_{ii} \phi_i + H_{b}^{T} \phi_b. \tag{3.74}
\]

Setting the partial derivatives to zero we establish a set of algebraic equations which can be written in a matrix form as:

\[
\begin{bmatrix}
H_{bb} & H_{bi} \\
H_{b}^{T} & H_{ii}
\end{bmatrix}
\begin{bmatrix}
\phi_b \\
\phi_i
\end{bmatrix}
= \begin{bmatrix}
\lambda \\
0
\end{bmatrix}. \tag{3.75}
\]

5. Solution of the set of algebraic equations which gives the solution of the potential.

From the second part of Equation (3.75):

\[
\begin{bmatrix}
H_{b}^{T} & H_{ii}
\end{bmatrix}
\begin{bmatrix}
\phi_b \\
\phi_i
\end{bmatrix}
= 0, \tag{3.76}
\]

we have:

\[
\phi_i = -H_{ii}^{-1} H_{b}^{T} \phi_b. \tag{3.77}
\]

The formal solution of the problem is therefore given by:

\[
\phi = \begin{bmatrix}
\phi_b \\
-H_{ii}^{-1} H_{b}^{T} \phi_b
\end{bmatrix}. \tag{3.78}
\]

The vector \( \lambda \) of Lagrange multipliers has a physical interpretation. It is the vector of charges needed on the boundary nodes to maintain the potential inside (the inside nodes are charge free). Setting \( \lambda = \delta_b \), the vector of the boundary node charges, we can rewrite Equation (3.75) as:

\[
\begin{bmatrix}
H_{bb} & H_{bi} \\
H_{b}^{T} & H_{ii}
\end{bmatrix}
\begin{bmatrix}
\phi_b \\
\phi_i
\end{bmatrix}
= \begin{bmatrix}
\delta_b \\
0
\end{bmatrix}. \tag{3.79}
\]

3.7 Capacitance network

We can determine the potential distribution, as has been shown in the last section, by solving Equation (3.76) using a standard method. From the point of view of capacitance extraction, however, it is more interesting to find the capacitance matrix
3.7 Capacitance network

and its corresponding capacitance model.

Let $H^{(e)}$ be the $4 \times 4$ capacitance matrix of the capacitance network spanned on the tetrahedral element.

The matrix $H^{(e)}$ gives the relationship between the charges and the potentials:

$$\delta^{(e)} = H^{(e)} \Phi^{(e)} ,$$  \hspace{1cm} (3.80)

with $\delta^{(e)} = [ \delta_1 \ \delta_2 \ \delta_3 \ \delta_4 ]^T$ and $\Phi^{(e)} = [ \phi_1 \ \phi_2 \ \phi_3 \ \phi_4 ]^T$ the node charges and node potentials, respectively.

Writing the matrix $H^{(e)}$ as:

$$H^{(e)} = \begin{bmatrix}
    h_{11} & h_{12} & h_{13} & h_{14} \\
    h_{12} & h_{22} & h_{23} & h_{24} \\
    h_{13} & h_{23} & h_{33} & h_{34} \\
    h_{14} & h_{24} & h_{34} & h_{44}
\end{bmatrix} ,$$  \hspace{1cm} (3.81)

we can construct a capacitive model of the tetrahedral finite element, in which each edge between nodes $i$ and $j$ corresponds to a capacitance $h_{ij}$. The equivalent capacitive network corresponding to a tetrahedral element is shown in Figure 3.9.

For the assembled problem, we collect the models of all single elements and we join them according to the continuity conditions in nodes. The relation between the node charges and the node potentials can be written in matrix form as:

$$\delta = H \Phi ,$$  \hspace{1cm} (3.82)

where $\Phi$ is the vector of all node potentials, and $\delta$ the vector of all node charges with non-zero entries only for the boundary nodes, since the internal nodes are charge free.

Partitioning Equation (3.82) gives:

$$\begin{bmatrix}
    H_{bb} & H_{bi} \\
    H_{ib} & H_{ii}
\end{bmatrix} \begin{bmatrix}
    \phi_b \\
    \phi_i
\end{bmatrix} = \begin{bmatrix}
    \delta_b \\
    0
\end{bmatrix} .$$  \hspace{1cm} (3.83)

**Figure 3.9.** Equivalent capacitive network corresponding to a tetrahedral element.
Elimination of \( \phi_i \)'s from Equation (3.83) yields:

\[
[H_{bb} - H_{bi}H_{ii}^{-1}H_{ib}]\phi_b = \delta_b.
\]  

(3.84)

The matrix \( H^{(b)} \), given by:

\[
H^{(b)} = H_{bb} - H_{bi}H_{ii}^{-1}H_{ib}
\]

(3.85)

is the capacitance matrix after the internal nodes are reduced. It describes the capacitance model established between all pairs of the boundary nodes. This is the solution of the capacitance modeling problem.

Elimination of the \( \phi_i \)'s can be done using the classical techniques, e.g. Gaussian elimination. Simply speaking, we eliminate from the matrix \( H \) the rows and columns corresponding to the internal nodes. In the network representation, this exhibits itself as the elimination of a node based on a star-triangle transformation for that node. We illustrate the elimination of a node in Figure 3.10.

![Figure 3.10](image)

**Figure 3.10.** The network interpretation for the elimination of a row/column \( m \) from the matrix \( H \).

When eliminating the node \( m \) from the network, the new capacitance \( h_{ij}' \) between the nodes \( i \) and \( j \) becomes:

\[
h_{ij}' = h_{ij} + \frac{h_{im}h_{mj}}{h_{mm}},
\]

(3.86)

where

\[
h_{mm} = \sum_{i=1}^{N} h_{mi}
\]

(3.87)

is the sum of the capacitances connected to the node \( m \). The elimination of the internal nodes may be done after the entire network is constructed, but for extraction purposes and the scanline concept, for details see Section 8.3.1, it is more appealing to eliminate the nodes successively during the network construction.
3.8 Properties of the capacitance matrix

A variety of properties of the capacitance matrix can be deduced by referring to various physical principles.

First, Green's theorem for the capacitance problem shows that the resulting capacitance matrix $H$ is symmetric:

$$h_{ij} = h_{ji} \quad (3.88)$$

Next, suppose that all the applied potentials on the boundary are the same. In this case the electric field vanishes identically, and there are no field lines. Thus one may conclude:

$$\sum_{j=1}^{N} h_{ij} = 0 \quad \text{for } j = 1, 2, \ldots, N. \quad (3.89)$$

From conservation of the electric charge we have that, independent of the values of the applied potentials, the sum of all the charges must vanish. This condition requires that:

$$\sum_{i=1}^{N} h_{ij} = 0 \quad \text{for } j = 1, 2, \ldots, N. \quad (3.90)$$

From properties (3.89) and (3.90) of the capacitance matrix we can conclude that the matrix $H$ is singular and cannot be inverted. This reflects the fact that there is no absolute zero of potential, and therefore specifying of the charges does not uniquely determine the potentials.

We will show also that the matrix $H$ is positive semi-definite. The principle of linear superposition gives the charge $\delta_i$ associated with the $i^{th}$ node as:

$$\delta_i = \sum_{j=1}^{N} h_{ij} \phi_j. \quad (3.91)$$

The power that is dissipated in the dielectric medium is given by:

$$\sum_{i=1}^{N} \phi_i \delta_i, \quad (3.92)$$

and must be non-negative. As a result the capacitance matrix must be positive semi-definite, this means:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} \phi_i h_{ij} \phi_j \geq 0, \quad (3.93)$$

for any set of applied potentials.
For the last property we analyze the sign of the entries of the capacitance matrix. Suppose that the \( i^{th} \) node is raised to a positive potential \( \phi_i > 0 \), while all the other nodes are kept at the zero reference potential. In this case the field lines will go into the \( i^{th} \) node and out of all the other nodes. For the capacitance matrix this means that:

\[
    h_{ij} \leq 0 \quad \text{for } i \neq j, \quad (3.94)
\]

and

\[
    h_{ii} \geq 0. \quad (3.95)
\]

### 3.9 Conclusions

In this chapter we have discussed the applicability of the finite element method to the capacitance modeling problem in IC’s. We have given the theoretical and mathematical background of the FEM. We have also shown how the equivalent capacitive models can be derived for the finite elements by using the FEM.
Bibliography


Chapter 4

THE HYBRID ELEMENT METHOD

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4.1 Introduction

In advanced chip technologies complex dielectric structures are present which have a significant influence on capacitance values. Inside these structures the permittivity of the dielectric medium may vary irregularly. This can be the case e.g. in places where the planarization is not perfect or the stratification is disturbed by the presence of features.

To obtain accurate capacitance values for a given geometry, the best practical way is to use a detailed numerical modeling technique. Our main goal will be to derive an algorithm that incorporates a boundary element solution of the capacitance problem and special treatment of dielectric disturbances of the medium, such that complex 3D IC structures can be handled in an efficient manner.

There are two fundamental methods for the numerical computation of capacitance values:

- the finite element method (FEM) which is based on the differential form of the equations in electrostatics and solves the potential throughout the space;
The hybrid element method

- the boundary element method (BEM), often called an integral-equation method, which is based on the integral form of the electrostatics equations and as solution gives the charge density.

Each of methods has certain advantages and disadvantages and in many cases they are complementary.

As disadvantages of the FEM we count:

- a requirement for the generation is a finite element mesh which has to fill all space in consideration, and therefore the method needs an extremely large number of elements to obtain a good accuracy;
- the potential field must be numerically differentiable;
- the method requires closed boundaries;

But except these drawbacks the FEM offers us advantages which reflect in the following properties:

- the matrix of coefficients of the linear system is extremely sparse;
- the few elements which have non-zero values are easy to compute;
- the matrix is inherently symmetric;
- because of the use tetrahedral elements, the method can handle complex geometries in a natural and straightforward manner;
- the method is adaptable to nonlinear fields.

The boundary element method has the following advantages:

- the variables for which one solves are the charge densities form a much smaller set;
- the charge is present only on the surface of the conductors and at the dielectric boundaries;
- as a consequence of the above we need to discretize only those surfaces on which a charge is present and not the whole 3D space;
- for solving the 3D modeling problem we have only to discretize finite 2D surfaces;
- a number of variables appearing in this method is smaller than in the FEM methods;
4.1 Introduction

- the matrix is (usually) symmetric;
- a diagonal dominance is assured;
- boundaries can be open or closed.

As disadvantages of the BEM we can count:

- the coefficient matrix of the linear system is full;
- the cost of evaluating the entries of the matrix is high;
- the method requires a big computational effort for complex dielectric geometries;
- an integration over singularities is required;
- there are difficulties with the application of this method to nonlinear fields.

As we can see from the specification presented above, where one method has its weak points, the other is strong. Thus it is useful to combine these two methods to obtain efficient accurate models for the capacitance modeling problem.

The hybrid modeling can be tackled in many ways. The most appealing approach is to couple the finite element method and boundary element method, while maintaining the best features of both. Some research on this subject has been done already in other contexts like geophysics [Lee 81], [Gupta 87], electromagnetism [Salon 82], [Salon 85], structural mechanics, acoustics, elastostatics [Brebbia 79] or thermal analysis [Pichon 91].

Most of these methods attempt to solve the modeling problem of the local inhomogeneities (regions which have to be treated in detail) embedded in a uniform or layered medium. A closed inhomogeneous domain is modeled by using the finite element method, while the outside of this domain is modeled by the boundary element method. Both grids coming from the FEM and the BEM coincide at the boundary of the restricted region. Moreover, there are imposed continuity conditions at the boundary. In the known hybrid techniques an iteration scheme between solutions, which come from different equations used in the specified regions, is applied to assure continuity at the boundary. The iterative process is repeated until changes in the boundary values become insignificant.

Another approach assumes that the total field consists of the "background" potential field, i.e. the field that would be present if the layered medium would be uniform, and the "scattered" field associated with the disturbance. Then by taking care about matching boundary conditions we can directly determine both components of the total potential. But for the purpose of model construction, the expressions obtained from a direct solution are not attractive from the point of view of physical interpretation. It is very difficult to build any sensible model.
The direct hybrid method described in this dissertation seems to be, as far as our knowledge goes, superior to the other hybrid methods. The hybrid approach presented in this chapter incorporates a multi-layer Green's function to include the effects of the bound charges at the infinite planar dielectric interfaces and special treatment of the finite dielectric interfaces. We call this the "direct hybrid method", because it finds an accurate approximation for field problems in which different parts of the 3D space are modeled with different methods, namely bounded and restricted "inside" domains are modeled using finite elements, while the "outside" open domain is modeled using boundary elements. The difficulty of the hybrid modeling problem is the matching boundary conditions between specified regions.

The classical methods try to solve this problem using the point collocation method [Brebbia 84] but the resulting capacitance matrix is not symmetric whereas all passive physical systems have a symmetric system matrix. In the case described in this dissertation matching can be done directly by solving a hybrid system of equations i.e. in which quantities of different dimensions like potentials and charges appear [Nowacka 96a], [Nowacka 96b]. The solution of this system of equations results in the global capacitance model which is our ultimate goal.

The main advantages of the hybrid method proposed in this dissertation are:

- a direct solution without an iterative procedure;
- an attractive physical interpretation resulting in the relevant capacitance model.

In this chapter we introduce our new hybrid method to solve the capacitance modeling problem. We shall work with a purely capacitive situation, i.e. with a domain in which the dielectric permittivity varies irregularly and which needs to be modeled in detail.

### 4.2 Physical situation

We model the integrated circuit overall as a 3D stratified medium in which a number of ideal conductors is placed, and in which also subregions occur where the permittivity varies irregularly. This is the case e.g. in places where the stratification is disturbed due to, for example, imperfect planarization, presence of voids or cavities filled with different dielectric. As illustration of this we refer to the cross-section of Figure 4.1 in which some of these causes are shown. The key concept of our technique is to use the BEM for parts of IC exhibiting regularity, and the FEM for the bounded localized irregular regions [Nowacka 96a], [Dewilde 96].

To better illustrate this idea we show in Figure 4.2 a simplified situation for the capacitance problem. The unbounded dielectric half-plane bordered at the bottom
4.2 Physical situation

Here, we consider situations such as the ground plane, where we imagine that the Green's function is constant. We focus on the surface of a perfectly conducting ground plane and consider a single conductor floating in the region by the FEM.

Figure 4.1. Cross-section of a typical IC structure showing the possible causes for the disturbance of the stratification. Courtesy of Philips Research Labs, Eindhoven, The Netherlands.

![Cross-section of an IC structure](image)

Figure 4.2. The sketch for the capacitance situation.

by a perfectly conducting ground plane is shown. The system of $M$ conductors and region in which the permittivity varies are floating in the medium.

We split the domain of our interest into three regions as shown in Figure 4.3.

The "inside" region is the region depicted in Figure 4.3 as the domain $\Omega_2$ and the FEM will be applied there.

In order to specify the "inside" region we must introduce its artificial boundary which we call the boundary interface. It is as if the boundary consists of two coinciding charge layers (infinitely close to each other), one inside and one outside. We require the potential on the inside and the outside layer of the boundary interface to match well, and the charges to compensate each other - the layers should have opposite charges. If there is an exact match Maxwell's equations will be satisfied exactly also, due to a linearity.

We assume that the boundary interface runs through a region of constant permittivity, i.e. there is no discontinuous change of the dielectric permittivity across the
The hybrid element method described in this chapter is to be, as far as our knowledge goes, the most direct solution of the electromagnetic scattering problem. The hybrid approach presented in this chapter is designed to include the effects of the specific structure and special treatment of the electrical field. The hybrid method is based on the concept of the hybrid model, which is a combination of the finite element method (FEM) and the method of moments (MOM). The hybrid model is an attractive solution for electromagnetic scattering problems because it combines the advantages of both methods: the FEM is well suited for solving problems with complex geometries, while the MOM is efficient for problems with large numbers of unknowns.

The main advantages of the hybrid method proposed in this chapter are:

1. A direct solution without extensive procedures.
2. An attractive physical interpretation of the results in terms of capacitance model.
3. This chapter introduces the hybrid model's application to the scattering problem. We shall work with the particular problems of scattering from a dielectric object in an infinite medium. In the next section, we will present the details of the model's application to the scattering of plane waves by a dielectric object in a uniform medium.

### Figure 4.3. Partitioning of the modeled domain.

The "outside" region is the complete hemisphere above the ground plane minus the interior of the region where the FEM is used, namely the "inside" region. The boundaries of the "outside" region are thus given by the conductors, the ground plane, the boundary at infinity and the boundary of the "inside" region. We can neglect the boundary at infinity, since we assume that the potential and the electrical boundary.
4.3 Discretization

The "inside" region is decomposed into tetrahedrons. The bounding interface consists then of a mesh of triangular boundary elements. On the surface of conductors we also place a triangulation mesh. There may be conductors carrying charges and potentials in both regions. This happens when the conductor crosses the "inside" region. The conductor mesh should in such a case be consistent with the mesh of tetrahedrons. If some conductors cross boundaries between the regions, the "outside" conductor mesh should be confined to the "outside" region so that surfaces on which the charge is present will be represented only once, i.e. in the boundary integral equation for the "outside" region. Otherwise there are no interfacing problems at the location of conductors.

4.4 Interpolation

In the "inside" region the potential is approximated by linear splines:

$$\Phi(x, y, z) = \sum_{k=1}^{N} f_k(x, y, z) \phi_k, \quad (4.1)$$
with $\phi_k$'s the node potentials and $f_k$'s the conjoint shape functions assigned to the nodes of the tetrahedrization mesh.

The potential on finite elements in the “inside” region, which have a face in common with the boundary interface determines the form of the interface charge layer. The charge on the interface boundary is constant in each face, since $\nabla \Phi$ is constant in the interior of each finite element.

By virtue of Gauss’s law the charge is defined as:

$$\sigma(q) = k(q) \frac{\partial \Phi(q)}{\partial n_q}, \quad (4.2)$$

which can be expressed as:

$$\sigma(q) = k(q)[\nabla_q \Phi(q) \cdot n_q]. \quad (4.3)$$

The gradient $\nabla_q \Phi$ of the linear potential on the tetrahedral finite elements adjacent to the boundary is then constant and the charge determined by the gradient is constant too.

The potential in the “outside” region is continuous and determined by the boundary integral equation:

$$\frac{1}{2} \Phi(p) + \int_{q \in S} \Phi(q) k(q) \frac{\partial G(p, q)}{\partial n_q} dq = \int_{q \in S} G(p, q) \sigma(q) dq. \quad (4.4)$$

Discretizing the charge $\sigma(q)$ by using constant shape functions, one obtains the following approximation of the potential for a point $p$ on the conductor:

$$\frac{1}{2} \Phi(p) + \sum_{q \in S} \Phi(q) k(q) \frac{\partial G(p, q)}{\partial n_q} dq = \sum_{q \in S} G(p, q) \sum_{i=1}^{N} \sigma_i f_i(q) dq. \quad (4.5)$$

### 4.5 Statement of the hybrid modeling problem

From the previous chapters we know how to construct the capacitive models for a given discretization and given shape functions in the “outside” and “inside” regions. The problem we consider here is the derivation of a good circuit model for the interface boundary which we consider as two-layered with the charges of the outside and inside layer compensating each other - assuming that there is no discontinuous change of the dielectric constant across the boundary.

For constant shape functions in the “outside” region the capacitance model consists of the capacitances between each pair of the boundary elements lying on the conductor surface or on the bounding surface of the “inside” region. This model also includes the so-called “autocapacitances” which are the capacitances between the face and the reference. Often, the ground plane which is at the zero potential is
4.6 Direct hybrid field modeling

taken as the reference and then the “autocapacitance” is called the ground capacitance.

On the other hand, the FEM, which uses linear shape functions to approximate the potential, produces a model consisting of capacitances along the edges of the tetrahedral mesh of 3D finite elements.

Figure 4.5 shows the capacitive models, as they result from the BEM and the FEM individually. The “outside” capacitive model consists of capacitances between the centers of gravity of the faces and from each face to the reference. The “inside” capacitive model consists of capacitances between the nodes of the tetrahedrons (along the edges of the mesh). Of course the problem now appears how to connect the models of the two different regions and what kind of boundary constraints we must impose on the boundary of the “inside” region to obtain a good circuit model for the boundary between the two regions.

We wish to connect the inside and outside models using a circuit which is non-dynamic, lossless and reciprocal. The circuit needed should moreover have the property that the average potentials should be the same at both sides and charges inside and outside should compensate each other. The only electrical circuit which satisfies these properties is a generalized ideal transformer, see [Belevitch 68]. The concept of modeling the interface between the two regions with an ideal transformer has been explained in detail in [Nowacka 96a], [Nowacka 96b].

4.6 Direct hybrid field modeling

We model the “outside” and “inside” regions with the BEM and the FEM, respectively, as described in the previous chapters.
The hybrid element method

In order to obtain the definition of the transformer for the boundary between the regions we consider the triangulation mesh on the interface boundary shown in Figure 4.6.

For each face on the interface boundary we have:

**Outside**: an average potential $\Phi_i$ over a face $i$ and a constant charge $\sigma_i$;

**Inside**: a node potential $\phi_{\alpha}$ associated with a node $\alpha$ and an overall node charge $\delta_{\alpha}$.

For each triangular finite element on the boundary interface we determine the center of gravity. We decompose the triangle along the gravity lines into three subregions of the same area, namely $\frac{1}{3}$ of the triangle area. The gravity lines are defined as the lines connecting the nodes of the triangle with the middle of the opposite triangle edge. The generated subregions of the triangle connect as an irregular (non-planar) polytope around each node.

Referring by example to Figure 4.6, we distribute the “outside” charge on a face $i$ evenly over the three bounding nodes, yielding for the case shown:

$$\delta_{\alpha} = \frac{1}{3} [\sigma_1 + \sigma_2 + \ldots + \sigma_5] \quad (4.6)$$

This yields the global equation for the charges:

$$\delta_b = T \sigma_b \quad (4.7)$$

in which $\delta_b$ is the vector of node charges and $\sigma_b$ the vector of outside interface charges at the boundary interface. The matrix $T$ is such that $t_{ij}$ is $\frac{1}{3}$ if the $i^{th}$ node belongs to the $j^{th}$ face on the boundary interface, and zero otherwise. The matrix $T$ is sparse and can be understood as $\frac{1}{3}$ of the incidence matrix which relates the nodes of the mesh to triangular elements. For the potential at the boundary interface we assume that each $\Phi_j$ is in fact the average of the node charges pertaining
4.7 Solution of the potential

Let us now collect the equations relevant to each region of the modeled domain:

- the “outside” region,

\[
\begin{bmatrix}
\sigma_c \\
-\sigma_b
\end{bmatrix} =
\begin{bmatrix}
C_{cc} & C_{cb} \\
CT_{cb} & C_{bb}
\end{bmatrix}
\begin{bmatrix}
\Phi_c \\
\Phi_b
\end{bmatrix}
\]

(4.10)

with \(\sigma_c\) and \(\Phi_c\) the conductor charges and potentials, respectively, and the minus sign on \(-\sigma_b\) due to the transformer sign convention and the compensation of the charges at the boundary interface between the regions modeled by the BEM and the FEM;

- the “inside” region,

\[
\delta_b = H\phi_b
\]

(4.11)

- the boundary interface,

\[
\delta_b = T\sigma_b
\]

(4.12)

\[
\Phi_b = T^T\phi_b
\]

(4.13)

To obtain the multiconductor capacitance matrix we proceed as follows [Nowacka 96c]:

1. multiply the second equation of (4.10) by \(T\),

\[
\begin{bmatrix}
\sigma_c \\
T\sigma_b
\end{bmatrix} =
\begin{bmatrix}
C_{cc} & C_{cb} \\
CT_{cb} & TC_{bb}
\end{bmatrix}
\begin{bmatrix}
\Phi_c \\
\Phi_b
\end{bmatrix}
\]

(4.14)
2. use (4.12) to rewrite (4.14),
\[
\begin{bmatrix}
\sigma_c \\
-\delta_b
\end{bmatrix} = \begin{bmatrix}
C_{cc} & C_{cb} \\
TC_{cb}^T & TC_{bb}
\end{bmatrix} \begin{bmatrix}
\Phi_c \\
\Phi_b
\end{bmatrix}
\] (4.15)

3. use (4.13) in (4.15),
\[
\begin{bmatrix}
\sigma_c \\
-\delta_b
\end{bmatrix} = \begin{bmatrix}
C_{cc} & C_{cb}^T \\
TC_{cb}^T & TC_{bb}^T
\end{bmatrix} \begin{bmatrix}
\Phi_c \\
\phi_b
\end{bmatrix}
\] (4.16)

4. use (4.11) in (4.16),
\[
\begin{bmatrix}
\sigma_c \\
-H\phi_b
\end{bmatrix} = \begin{bmatrix}
C_{cc} & C_{cb}^T \\
TC_{cb}^T & TC_{bb}^T
\end{bmatrix} \begin{bmatrix}
\Phi_c \\
\phi_b
\end{bmatrix}
\] (4.17)

5. reorder (4.17),
\[
\begin{bmatrix}
\sigma_c \\
0
\end{bmatrix} = \begin{bmatrix}
C_{cc} & C_{cb}^T \\
TC_{cb}^T & (TC_{bb}^T + H)^{-1}TC_{cb}^T
\end{bmatrix} \begin{bmatrix}
\Phi_c \\
\phi_b
\end{bmatrix}
\] (4.18)

6. assuming that \((TC_{bb}^T + H)\) is invertible, we eliminate \(\phi_b\) from (4.18)
\[
\sigma_c = (C_{cc} - C_{cb}^T(TC_{bb}^T + H)^{-1}TC_{cb}^T)\Phi_c
\] (4.19)

\((TC_{bb}^T + H)\) will be invertible when the system is properly grounded, the “inside” region is not grounded but it becomes grounded via transformers (the resulting matrix is non-singular);

7. apply the incidence matrix \(A\) relating the boundary elements to conductors on (4.19),
\[
C_s = A^T C_H A
\] (4.20)
where:
\[
C_H = C_{cc} - C_{cb}^T(TC_{bb}^T + H)^{-1}TC_{cb}^T
\] (4.21)

and \(C_s\) is the short circuit capacitance matrix we sought for.

The final result is in closed form but will not be computed in this way, as we can eliminate nodes “on the fly” and obtain reduced models at less computational cost. We discuss this in more detail in Chapter 8, Section 8.3.1.
4.8 Model construction

As mentioned, the matrix $T$ corresponds to a transformer winding matrix of an ideal multiport transformer.

The block structure of our model consists then (as shown in Figure 4.7) of:

- the capacitance model of the "outside" region described by the matrix $C$ and consisting of the capacitances between each pair of the boundary faces, including the capacitances to the ground plane;
- the capacitance model of the "inside" region described by the matrix $H$ and consisting of the capacitances along the edges of the mesh of 3D tetrahedral finite elements;
- the generalized ideal transformer with the winding matrix $T$ which couples the "inside" and "outside" models at the boundary interface.

Let us concentrate on the transformer model at the boundary interface. The schematic circuit model of the interface transformer is presented in Figure 4.8.

![Figure 4.7. A block structure of the hybrid model.](image)

**Figure 4.7.** A block structure of the hybrid model.

**Figure 4.8.** The schematic circuit model of the transformer. Here $T$ is the winding matrix.

Here, the $\Phi_h$ and $\sigma_h$ represent interface potentials and charges, $\phi_h$ and $\delta_h$ the node potentials and charges at the interface boundary. Taking a closer look at the trans-
former we can represent the matrix $T$ as an equivalent circuit model displayed in Figure 4.9.

![Figure 4.9. The appearance of the transformer which models the boundary interface.](image)

Focusing on a single boundary face on the interface boundary we see that the transformer model is as that shown in Figure 4.10.

Equation (4.21) gives a closed form solution of the capacitance problem, but it is not a good way to calculate the capacitance matrix $C_H$ from the point of view of circuit extraction. It is more interesting and more appealing to see how the network changes in the course of introduction and elimination of the transformers [Nowacka 96c]. To visualize this process we consider a part of the network associated with the $a^{th}$ face lying on the boundary interface, see Figure 4.11.

The behavior of a single capacitor is described by a differential equation of the first order:

$$i(t) = \frac{\partial q(t)}{\partial t} = C \frac{\partial u(t)}{\partial t} \quad (4.22)$$
4.8 Model construction

Figure 4.10. The equivalent transformer model of the triangular face at the boundary interface.

Figure 4.11. A part of the network associated with the face at the boundary interface.

with $C$ the capacitive value, $i(t)$ the current, $u(t)$ the voltage and $t$ the time. Referring to the Laplace transform we denote by $s$ the operator $\frac{\partial}{\partial t}$. Equation (4.22) can then be written as:

$$i = sC \cdot u$$

(4.23)
here, \( i \) is the current flowing through the capacitive element, \( u \) is the voltage on the element. The network equations for the network shown in Figure 4.11 are:

- the current distribution for the \( a^{th} \) face:
  \[
  j_1 = sC_1(U_1 - U_a) \\
  j_2 = sC_2(U_2 - U_a) \\
  \vdots \\
  j_k = sC_k(U_k - U_a)
  \]  
  (4.24)

- Kirchhoff's current law for the \( a^{th} \) face:
  \[
  j_1 + j_2 + \ldots + j_k = sC_g U_a + i_a
  \]  
  (4.25)

- the transformer equations for the \( a^{th} \) face:
  \[
  U_a = \frac{1}{3}(u_1 + u_2 + u_3) \\
  i_1 = i_2 = i_3 = -\frac{1}{3}i_a
  \]  
  (4.26)
  (4.27)

We express the “face” current and “face” voltage as:

\[
  i_a = j_1 + j_2 + \ldots + j_k - sC_g U_a \\
  U_a = \frac{1}{3}(u_1 + u_2 + u_3)
  \]  
  (4.28)  
  (4.29)

and eliminate them from the set of network equations. Hence:

\[
  -3i_1 = j_1 + j_2 + \ldots + j_k - sC_g \frac{1}{3}(u_1 + u_2 + u_3) \\
  -3i_2 = j_1 + j_2 + \ldots + j_k - sC_g \frac{1}{3}(u_1 + u_2 + u_3) \\
  -3i_3 = j_1 + j_2 + \ldots + j_k - sC_g \frac{1}{3}(u_1 + u_2 + u_3) \\
  j_1 = sC_1[U_1 - \frac{1}{3}(u_1 + u_2 + u_3)] \\
  j_2 = sC_2[U_2 - \frac{1}{3}(u_1 + u_2 + u_3)] \\
  \vdots \\
  j_k = sC_k[U_k - \frac{1}{3}(u_1 + u_2 + u_3)]
  \]  
  (4.30)  
  (4.31)  
  (4.32)  
  (4.33)  
  (4.34)  
  (4.35)
writing the last set of equations in a matrix form we have:

\[
\begin{bmatrix}
  j_1 \\
  j_2 \\
  \vdots \\
  j_k \\
  i_1 \\
  i_2 \\
  i_3
\end{bmatrix}
\begin{bmatrix}
  sC_1 \\
  sC_2 \\
  \vdots \\
  sC_k \\
  -\frac{1}{3}sC_1 \\
  -\frac{1}{3}sC_2 \\
  -\frac{1}{3}sC_k
\end{bmatrix}
\begin{bmatrix}
  U_1 \\
  U_2 \\
  \vdots \\
  U_k \\
  u_1 \\
  u_2 \\
  u_3
\end{bmatrix}
\]

(4.36)

Here the capacitance \( C_t \) is defined as:

\[
C_t = C_1 + C_2 + \ldots + C_k + C_g
\]

(4.37)

The matrix equation (4.36) describes the network of Figure 4.11 after the transformers are eliminated. The corresponding network is shown in Figure 4.12.

Figure 4.12. The reduced network after the transformers are eliminated.

The circuit model contains negative capacitances spanned on the boundary nodes of the interface. They are eliminated, however, once the capacitive network of the “inside” region is connected and Gaussian elimination of the boundary interface nodes is applied.

The resulting model is purely capacitive with capacitances between each pair of conductor faces. The derivation of the multiconductor capacitances is straightforward, see Section 2.3.5.
In the next chapter we will show that the transformer model is correct and converges one order of magnitude better than the BEM and the FEM themselves. In the following chapters we will also explain how the transformer model can be efficiently incorporated in the capacitance extraction system.

4.9 Conclusions

In this chapter we have introduced a new hybrid element method which combines the BEM with the FEM. We have shown how the capacitive models obtained by these methods separately, can be combined by an ideal generalized transformer at the boundary between the regions where the methods are applied. We have also presented the derivation of the multiconductor capacitances which are obtained by eliminating the transformers.
Bibliography


Chapter 5

CONVERGENCE OF THE HEM

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5.1 FEM - measures, error estimation and nature of its convergence

There are three main sources of error in a finite element solution:

1. errors due to approximation of the domain - the discretization error;
2. errors due to the approximation of the solution (method error);
3. errors due to numerical computation (e.g. numerical integration and round-off errors in a computer).

The estimation of these errors is, in general, not a simple matter. We focus here only on the discretization error which is due to the use of approximate solutions that contain only a finite number of terms. This approximation is the main principle of the FE method and hence is generally the most significant determinant of the accuracy of an FE solution.
If the exact solution in domain $\Omega$ is $\Phi(p)$ and the approximate solution is $\tilde{\Phi}(p)$, then we are interested in the pointwise error,

$$E(p) = |\Phi(p) - \tilde{\Phi}(p)|$$ (5.1)

which is the difference (or distance) between $\Phi$ and $\tilde{\Phi}$ for some $p$.

We want to estimate the error of the approximation and to determine the nature of its convergence in terms of the size of discretization of the finite element mesh.

The estimation of the error can be done by use of different measures and thus we can distinguish the following types of convergence:

- pointwise convergence;
- uniform convergence;
- convergence in the mean;
- convergence in energy.

The pointwise error is the difference of $\Phi$ and $\tilde{\Phi}$ at each point of the domain. We expect that the sequence of approximate solutions $\Phi_n$ (n indicates the number of finite elements) will converge indefinitely:

$$|\Phi(p) - \Phi_n(p)| \to 0 \text{ as } n \to \infty$$ (5.2)

for all points $p$ in the domain $\Omega$.

This kind of convergence we call pointwise. It describes the approximate solution as approaching arbitrarily close to the exact solution, at each point of the domain, when the number of finite elements increases indefinitely.

But we can also use the sup-norm to estimate the error. The difference of $\Phi$ and $\tilde{\Phi}$ is then the maximum of all absolute values of the differences of $\Phi$ and $\tilde{\Phi}$ in the domain $\Omega$:

$$\|\Phi - \tilde{\Phi}_n\|_\infty = \max_{p \in \Omega} |\Phi(p) - \tilde{\Phi}(p)|$$ (5.3)

The uniform convergence is associated with this measure and requires,

$$\|\Phi - \tilde{\Phi}_n\|_\infty \to 0 \text{ as } n \to \infty$$ (5.4)

This is a bit stronger than pointwise convergence since it requires a uniform rate of convergence at every point in the domain.

More generally used measures of the difference of two functions are the $L^2$ norm and the energy norm. They involve an average of a function of the pointwise error over the domain. For any square-integrable functions $\Phi$ and $\tilde{\Phi}_n$, defined on the domain $\Omega$, the two norms are defined by:

For $f, g$ square-integrable on $\Omega$,

$$\|f - g\|_2 = \left( \int_{\Omega} |f - g|^2 \right)^{1/2}$$

and

$$\|f - g\|_E = \left( \sum_{i} \left( \int_{\Omega_i} |f - g|^2 \right)^{1/2} \right)$$
5.2 Conditions for the convergence of the FEM

5.2 Conditions for the convergence of the FEM

The convergence theorems require the approximating functions to satisfy the completeness and continuity conditions. The completeness condition is fundamental and ensures that it is possible for a sequence of approximate solutions, for a refined finite element mesh, to get arbitrarily close to the exact solution. This condition requires that the approximating functions belong to an infinite sequence of functions such that a linear combination of an arbitrarily large but finite number of the approximating functions is capable of approximating the exact solution arbitrarily close. The closeness is measured by the energy error being an integral over the domain $\Omega$ of a function of the pointwise error:

$$
\text{Energy error} = \int_{\Omega} |\nabla_p (\Phi(p) - \tilde{\Phi}(p))|^2 \, dp
$$

The approximate solutions can then converge to the exact solution with respect to the energy, i.e. the energy error can be made as close to zero as desired.

The expression for the energy error is meaningful only if the gradient $\nabla_p \tilde{\Phi}(p)$ is well-defined, i.e. the gradient of $\tilde{\Phi}(p)$ exists. This in turn requires $\tilde{\Phi}(p)$ to be continuous and at least continuous and piece-wise differentiable. This is the source of the continuity condition which is related to the boundaries between elements. Namely, the potential $\tilde{\Phi}(p)$ and its derivative are required to be continuous. The continuity condition is not necessary for convergence. It ensures that the discontinuities at the interelement boundaries are not severe enough to introduce errors. The condition can be relaxed, if the errors that are introduced decrease to zero fast.
enough as the mesh is refined and the convergence to the exact solution still occurs. If both the completeness and continuity conditions are satisfied then the convergence is ensured. Simply these two conditions are sufficient for convergence in energy.

First let us examine the completeness condition. A 3D polynomial has the general form (with \( a_0, a_1, \ldots, a_N \) coefficients),

\[
a_0 + a_1x + a_2y + a_3z + a_4x^2 + a_5y^2 + a_6z^2 + a_7xy + a_8xz + a_9yz + \ldots \tag{5.8}
\]

A complete linear polynomial contains the first four terms, the constant and three linear terms. Then the simplest form of the approximating shape function in the element is:

\[
\Phi^e(x, y, z) = a_0 + a_1x + a_2y + a_3z \tag{5.9}
\]

Let us now examine the continuity condition. In 3D space with tetrahedral finite elements the interelement boundary is a surface. In Chapter 3 we presented the standard derivation of the shape functions. Let us consider two adjacent tetrahedrons \((e)\) and \((f)\). They have a triangular face in common with nodes, say, 1, 2 and 3. The approximate potential \(\Phi^e\) in the element \((e)\) forms a (surface) 2D-manifold along the common face, i.e. between the node potentials \(\phi_1, \phi_2\) and \(\phi_3\). Since a surface is uniquely determined by values at three points, \(\Phi^e\) is uniquely determined along the common face by the values \(\phi_1, \phi_2\) and \(\phi_3\). Consequently, if the approximating function in the neighboring element \((f)\) assumes the same values \(\phi_1, \phi_2\) and \(\phi_3\), then \(\Phi^f\) would be the same surface along the common face, thereby establishing interelement continuity. As we can see, the purpose of assembly is to impose continuity at the nodes. In turn the continuity at the nodes produces continuity along the interelement boundaries.

### 5.3 Rate of convergence in FEM

As mentioned there are many different ways to measure the error of the finite element solution. The most convenient measure employed by convergence theorems is the energy measure. However, the pointwise error is usually of interest in practical applications.

We want to examine the error at some point \(p^* = (x^*, y^*, z^*)\) in the domain. The basic tool in our analysis is the Taylor’s series expansion. We expand both the exact solution and the approximate solution as a Taylor’s series, and we analyze the difference on the finite element, to assess the character of the error.

As it has been explained before we use a linear approximation in each element. The finite element solution in the element can then be expressed as:

\[
\Phi^e(x, y, z) = c_0 + c_1(x - x^*) + c_2(y - y^*) + c_3(z - z^*) \tag{5.10}
\]
5.4 The Galerkin boundary element method and its optimal solution

The Taylor's series expansion of the exact solution about the same point \( p^* \) is given by:

\[
\Phi^e(x, y, z) = a_0 + a_1(x - x^*) + a_2(y - y^*) + a_3(z - z^*) + O(h^2).
\]

(5.11)

Here, the remainder \( O(h^2) \) associated with the Taylor's series expansion is a function of \( h \) which is directly related to the size of the finite element.

The error associated with the finite element solution becomes:

\[
E(x, y, z) = a_0 + a_1(x - x^*) + a_2(y - y^*) + a_3(z - z^*) + O(h^2) - c_0 - c_1(x - x^*) - c_2(y - y^*) - c_3(z - z^*)
\]

(5.12)

It is assumed that for a fine enough mesh, \( a_i \approx c_i \) for \( i = 0, 1, 2, 3 \), so the constant and linear terms essentially cancel, and we arrive with:

\[
E(x, y, z) = O(h^2)
\]

(5.13)

In a similar fashion it can be shown that the pointwise error in the derivative of the potential is of order \( O(h) \).

In this section we considered the pointwise convergence and its rate. Similarly we will formulate the rate of convergence in energy. We say that the finite element solution \( \Phi \) converges in the energy norm to the true solution \( \Phi^e \) if,

\[
\|\Phi - \Phi^e\|_e \leq f(p)h^k \quad \text{for} \quad k > 0
\]

(5.14)

where \( f(p) \) is independent of \( \Phi \) and \( \Phi^e \) and \( k \) is the rate of convergence.

5.4 The Galerkin boundary element method and its optimal solution

In this section we show that a good approximation of the boundary charges on conductors produces a good approximation of the potential by integrating the source charges with the Green's function.

Let us consider a system of conductors. The surface of conductors is divided into a number of boundary elements, say \( N \). We approximate the charge density \( \sigma(q) \) by a set of constant shape functions. The approximate charge density then becomes:

\[
\tilde{\sigma}(q) = \sum_{i=1}^{N} \sigma_i f_i(q)
\]

(5.15)

Let the corresponding approximate potential be \( \tilde{\Phi} \). There will be a one-to-one relation between the field \( \Phi \) and the boundary source function \( \sigma(q) \) given by:

\[
\Phi(p) = \int_S G(p, q)\sigma(q) \, dS_q
\]

(5.16)
Since distances between potentials are measured by energy integrals, we want to define a similar measure for the source functions. To derive a suitable measure let us consider first two fields $\Phi_\eta$ and $\Phi_\xi$ and their boundary source functions $\sigma_\eta$ and $\sigma_\xi$. The fields $\Phi_\eta$ and $\Phi_\xi$ satisfy the Laplace equation and can be expressed by using the Green's function as:

$$\Phi_\eta(p) = \int_S G(p,q) \sigma_\eta(q) \, dS_q$$  \hspace{1cm} (5.17)$$

$$\Phi_\xi(p) = \int_S G(p,q) \sigma_\xi(q) \, dS_q$$  \hspace{1cm} (5.18)$$

Green's theorem applied to the potentials $\Phi_\eta$ and $\Phi_\xi$ gives:

$$\int_\Omega k(p) \nabla_\eta \Phi_\eta(p) \nabla_\xi \Phi_\xi(p) \, dp = \int_{S_p} k(p) \Phi_\eta(p) \frac{\partial \Phi_\xi(p)}{\partial n_p} \, dS_p$$  \hspace{1cm} (5.19)$$

The normal derivative of $\Phi_\xi$ can be expressed as:

$$\frac{\partial \Phi_\xi(p)}{\partial n_p} = \int_{S_q} \frac{\partial G(p,q)}{\partial n_p} \sigma_\xi(q) \, dS_q$$  \hspace{1cm} (5.20)$$

Substitution of (5.20) into (5.19) yields:

$$\int_\Omega k(p) \nabla_\eta \Phi_\eta(p) \nabla_\xi \Phi_\xi(p) \, dp = \int_{S_p} k(p) \Phi_\eta(p) \cdot \left[ \int_{S_q} \frac{\partial G(p,q)}{\partial n_p} \sigma_\xi(q) \, dS_q \right] \, dS_p$$  \hspace{1cm} (5.21)$$

From [Weber 54] we know that $k(p) \frac{\partial G(p,q)}{\partial n_p}$ acts as a Dirac impulse at point $p$ on the surface $S_q$. Using this property we evaluate (5.21) to:

$$\int_\Omega k(p) \nabla_\eta \Phi_\eta(p) \nabla_\xi \Phi_\xi(p) \, dp = \int_{S_p} \Phi_\eta(p) \sigma_\xi(q) \, dS_p$$

$$= \int_{S_p} \int_{S_q} G(p,q) \sigma_\eta(p) \sigma_\xi(q) \, dS_q \, dS_p$$  \hspace{1cm} (5.22)$$

Now we can define a proper inner product for the source functions as:

$$(\sigma_\eta, \sigma_\xi) = \int_\Omega k(p) \nabla_\eta \Phi_\eta(p) \nabla_\xi \Phi_\xi(p) \, dp$$  \hspace{1cm} (5.23)$$

The principle of the Galerkin method is that the field $\Phi$ satisfying the Laplace equation with the boundary conditions minimizes the energy functional:

$$E(\Phi) = \int_\Omega k(p) \| \nabla_\eta \Phi(p) \|^2 \, dp.$$  \hspace{1cm} (5.24)$$

Let us define the energy error for $\Phi$ and $\tilde{\Phi}$ in the domain $\Omega$ (except the surface of conductors $S_c$),

$$E(\Phi(p) - \tilde{\Phi}(p)) = \int_{\Omega - S_c} k(p) \| \nabla_\eta (\Phi(p) - \tilde{\Phi}(p)) \|^2 \, dp$$

$$= \int_{\Omega - S_c} k(p) \left[ \nabla_\eta (\Phi(p) - \tilde{\Phi}(p)) \right] \cdot \left[ \nabla_\eta (\Phi(p) - \tilde{\Phi}(p)) \right] \, dp$$  \hspace{1cm} (5.25)$$
5.5 Convergence of the HEM

Using the inner product (5.23) for the source functions we write the energy error as:

\[ E(\Phi(p) - \Phi(p)) = \int_{S_i} \int_{S_o} G(p,q) [\sigma(p) - \bar{\sigma}(p)] \\
\times [\sigma(q) - \bar{\sigma}(q)] dS_p dS_q \]  
(5.26)

for potential \( \Phi(p) \) defined by:

\[ \Phi(p) = \int_{S_c} G(p,q) \sigma(q) dS_q \]  
(5.27)

and similarly for \( \Phi(p) \) with \( \bar{\sigma}(q) \).

Now we see that \( \Phi(p) \) and \( \Phi(p) \) will be close everywhere in 3D space if \( \sigma(q) \) and \( \bar{\sigma}(q) \) will be close on the surface of conductors. We conclude that a good approximation of the potential can be achieved by a good approximation of the boundary charges on conductors. From the theory of the Galerkin method we know that the error \( (\sigma - \bar{\sigma}) \) will be minimal if it is orthogonal to all shape functions used in approximate expression for \( \bar{\sigma} \).

5.5 Convergence of the HEM

5.5.1 Introduction

We base the determination of the parameters of an approximate potential \( \Phi_a \) on the property that \( \Phi_a \) will be close to the exact (real) potential \( \Phi \) when the total energy \( E_r = \int k || \nabla \Phi_a ||^2 d\Omega \) is minimal. We define the total energy as the sum of the energies in the “outside” and “inside” regions, provided appropriate boundary constrains are satisfied [Nowacka 96]. The boundary interface between the regions consists of a triangulation mesh. For the \( i^{th} \) face on the interface boundary we have from outside the charge \( \sigma_i \) and the average potential used in Galerkin BE method \( \Phi_i \). We can conceive \( \Phi_i \) as being attached to the center of gravity of a boundary triangle. The node potentials in the “inside” region are denoted by \( \phi_k \). As explained in the Chapter 3, a charge \( \delta_k \) may be attached to each of these nodes. It indicates the global capacitive charge attached to the node. When the system has been brought into the situation described, a flow of energy has taken place through the boundary interface. An amount of:

\[ \int_{S_b} \Phi_b(p) \sigma(p) dS_b \]  
(5.28)

has flowed through the boundary surface \( S_b \) towards the “inside” region, which has absorbed an amount given by:

\[ \sum_{k=1}^{N_b} \phi_k \delta_k \]  
(5.29)
where \( N_b \) denotes the number of the boundary nodes (since the internal nodes do not have a netto charge).

Our strategy for the construction of the model for the boundary interface is to:

- keep two energy quantities equal,

\[
\int_{S_b} \Phi_b(p) \sigma(p) \, dS_b \cong \sum_{k=1}^{N_b} \phi_k \delta_k
\]  

(5.30)

- make sure that the field on the outside and inside boundary layers match approximately;

- keep the magnitude of charges approximately equal.

The only model which satisfies all these requirements is the ideal transformer introduced in the previous chapter. The last two conditions are satisfied directly by the transformer equations at the interface boundary. The conservation of energy is ensured as desired too, since for the discretization used we have:

\[
\int_{S_b} \Phi_b(p) \sigma(p) \, dS_b = \sum_{k=1}^{N_{bf}} \Phi_k \sigma_k = \Phi_b^T \sigma_b = \phi_b^T T \sigma_b
\]

\[
= \phi_b^T \delta_b = \sum_{k=1}^{N_b} \phi_k \delta_k
\]  

(5.31)

where \( N_{bf} \) denotes the number of the boundary faces.

Our goal will be now to show that the approximate solution may be found by minimizing the sum of energies of the individual components of the field, assuming the transformer equations to be in force at the boundary interface. In the next paragraph we give the argument for quadratic convergence of the interface model constructed by our hybrid method and the linear convergence in energy of the hybrid method follows. We give only the arguments for the convergence of the model since a complete proof would entail complicated geometric properties beyond the scope of this thesis. However, the arguments are physically convincing and confirmed by experiments.

### 5.5.2 Convergence proof

Due to the first order discretization and the minimum energy principle, the BEM and the FEM converge linearly with the size \( (h) \) of the mesh. We claim that the HEM converges in the same way and that the disturbance introduced by the transformer (the discontinuity at the BEM-FEM interface) goes to zero as \( O(h^2) \). The classical Galerkin convergence proof is not directly applicable here because of the discontinuity of the field at the interface boundary between the 'outside' and 'inside' regions. This produces an essential singularity in the gradient of the field.
5.5 Convergence of the HEM

which turns out to be "removable", it contributes a negligible part to the total energy, namely a part that goes to zero as $O(h^2)$ when the mesh refines. Because of this fact, the solution may be found by minimizing the sum of energies $\mathcal{E}(\Phi_{in}) + \mathcal{E}(\Phi_{out})$ of the individual components of the field, assuming the transformer equations being forced at the interface boundary.

The convergence argument, of which we present here, proceeds in three steps as follows:

**Step 1** *Within the class of solutions constructed by us, some are close to the actual.*

One starts from the actual, true field $\Phi$ and deduces from it a discretization which follows the outside and the inside mesh and is otherwise close to $\Phi$, e.g. of $O(h)$. The key to the construction is the discretization on the BEM-FEM boundary. Starting from $\Phi_{in}$ and the discretization, we must choose:

- a discretization of charges $\sigma_c$ on the conductors as piecewise constant functions on a grid of surface triangles;
- charges $\sigma_b$ and average potentials $\Phi_b$ attached to the gravity centers of triangles on the surface of the outside boundary layer;
- charges $\delta_b$ and potentials $\phi_b$ on the boundary triangles of the inside bulk mesh.

Let us choose the $\Phi_b$'s to be equal to the average of the actual potential $\Phi_{in}$ over the boundary triangles. The $\phi_b$'s are then, themselves, averages of $\Phi_b$'s determined by the transformer equations. The $\phi_b$'s determine in turn the linear continuous spline potential in the bulk region which minimizes the energy $\mathcal{E}(\Phi_{in})$. This, in turn, determines a corresponding charge density $\delta_b$ which approximates the actual, when the inside mesh is fine enough, because the FE method converges. From $\delta_b$, a consistent system of face charges $\sigma_b$ may be deduced. This can be done by assigning to each $\sigma_b$, a part of the $\delta_b$ charge proportional to its participation in the triangle to which $\sigma_b$ belongs (conservation of charge). The resulting $\sigma_b$ will again be a good approximation of the local charge. Now, reverting to the outside field we invoke the approximation properties of the BE method according to which a good approximation of the boundary charges will produce a good approximation of the field by integration with the Green’s function. Hence, we can construct combinations $(\Phi_{in}, \Phi_{out})$ of the hybrid discretization type which are as close as desired to the actual field.

This shows the first point. It is instrumental in showing that the set of basis functions utilized by the hybrid method is actually "complete": it can approximate geometrically any continuous and piecewise differentiable field.
Step 2  The solution obtained by minimizing $E(\Phi_{in}) + E(\Phi_{out})$ is $O(h)$ away from a piecewise continuously differentiable field.

Suppose that we have a discrete field $(\Phi_{in}, \Phi_{out})$. Now we wish to construct a third field $\Phi_{in}$ which is continuous and piecewise differentiable but otherwise close to $(\Phi_{in}, \Phi_{out})$. Let us assume, without too much loss of generality, that the "inside" region has the form of a parallelepiped ($P_1$). Consider now a second parallelepipedum ($P_2$) surrounding the first one and with an $h$-thin layer between the two. Then the boundary interface consists of the two parallel surfaces separated by a $h$-thin layer. We modify the outside field slightly ($O(h)$) so that it meshes with $P_2$. $\Phi_{in}$ is continuous and piecewise differentiable inside $P_1$ while $\Phi_{out}$ has the same properties outside $P_2$. In the thin layer between the surfaces of $P_1$ and $P_2$, we make the field continuous as well by interpolating linearly between $\Phi_{in}$ and $\Phi_{out}$. This defines a field $\Phi_{inter}$ and its gradient:

$$\|\nabla \Phi_{inter}\| \approx \frac{\Phi_{out} - \Phi_{in}}{h}$$  \hspace{1cm} (5.32)

We show that the energy contribution of $\Phi_{inter}$ is negligible. An estimate of this energy is:

$$\int_{\text{bound. surface}} k\|\nabla \Phi_{inter}\|^2 dV \approx \int_{\text{bound. surface}} k\frac{\|\Phi_{out} - \Phi_{in}\|^2}{h^2} h dS_{\text{boundary}}$$  \hspace{1cm} (5.33)

We show first that (5.33) is $O(h)$ and then refine to $O(h^2)$. If $(\Phi_{out} - \Phi_{in}) \approx O(h)$ then this energy term will go to zero as $O(h)$ as well.

The transformer equations match the average outside potential $\Phi_{i}$ over a $i$-th boundary element to the average inside potential $\Phi_{i} = \frac{1}{3}(\phi_{i1} + \phi_{i2} + \phi_{i3})$ where $\phi_{i}$'s are the node potentials of the $i$th face. Assuming the mesh so small that also the outside potential can be considered to be (nearly) linear over a face, we may actually take the average outside potential over $i$th face to be (nearly) equal to the numerical average of the outside node potentials.

Let us take a local coordinate system, as depicted in Figure 5.1, whose origin is at one node of face $i$, and whose $x$ and $y$ axes follow the edges of the face. Expressing potentials to $O(h^2)$in the local coordinate system, we find over the $i$th face:

$$\Phi_{out}(x, y) = \phi_{i1} + x \frac{\partial \Phi_{out}}{\partial x}|_{(0,0)} + y \frac{\partial \Phi_{out}}{\partial y}|_{(0,0)} + O(h^2)$$  \hspace{1cm} (5.34)

$$\Phi_{in}(x, y) = \phi_{i1} + x \frac{\partial \Phi_{in}}{\partial x}|_{(0,0)} + y \frac{\partial \Phi_{in}}{\partial y}|_{(0,0)} + O(h^2)$$  \hspace{1cm} (5.35)
Equating the averages:

$$\Phi_{av} = \frac{1}{3} [\phi_{i1} + \phi_{i2} + \phi_{i3}] = \frac{1}{3} [\phi_{i1} + \phi_{i2} + \phi_{i3}] + O(h^2) \tag{5.36}$$

and putting

$$\frac{\partial \phi_{\text{out}}}{\partial x}_{(0,0)} \approx \frac{\phi_{i2} - \phi_{i1}}{a}, \quad \frac{\partial \phi_{\text{out}}}{\partial y}_{(0,0)} \approx \frac{\phi_{i3} - \phi_{i1}}{b} \tag{5.37}$$

e etc. ... we find:

$$\Phi_{in}(x, y) = \Phi_{av} + \left( \frac{x}{a} - \frac{1}{3} \right) (\phi_{i2} - \phi_{i1}) + \left( \frac{y}{b} - \frac{1}{3} \right) (\phi_{i3} - \phi_{i1}) + O(h^2) \tag{5.38}$$

$$\Phi_{out}(x, y) = \Phi_{av} + \left( \frac{x}{a} - \frac{1}{3} \right) (\phi_{i2} - \phi_{i1}) + \left( \frac{y}{b} - \frac{1}{3} \right) (\phi_{i3} - \phi_{i1}) + O(h^2) \tag{5.39}$$

The difference evaluates to:

$$\Phi_{in}(x, y) - \Phi_{out}(x, y) = \left( \frac{x}{a} - \frac{1}{3} \right) [(\phi_{i2} - \phi_{i1}) - (\phi_{i2} - \phi_{i1})] + \left( \frac{y}{b} - \frac{1}{3} \right) [(\phi_{i3} - \phi_{i1}) - (\phi_{i3} - \phi_{i1})] + O(h^2) \tag{5.40}$$

Assuming the field is continuous both in the inside and the outside region, and a mesh of $O(h)$ we see that $\Phi_{in} - \Phi_{out}$ is indeed also of $O(h)$ as announced, mainly due to the transformer equations, and hence (5.33) also is $O(h)$. 

**Figure 5.1.** The “outside” and “inside” potential over the $i^{th}$ face. Average potentials match to $\Phi_{av}$.
**Step 3** If the grids are refined, then the solution obtained by minimizing $\mathcal{E}(\Phi_{in}) + \mathcal{E}(\Phi_{out})$ converges to the true one. In this final step we show that the actual, true field $\Phi$ can be approximated as close as desired by a pair $(\Phi_{in}, \Phi_{out})$ which are hybrid discretizations of the type described earlier.

The convergence of the method now follows from the following final arguments. According to the Galerkin theory, all continuous, piecewise differentiable potential fields which match the boundary conditions have energy larger than the unique minimal field $\Phi_m$. When the mesh on the boundary is fine, then the energy $\mathcal{E}(\Phi_{out}) + \mathcal{E}(\Phi_{in})$ of the discretized field $(\Phi_{out}, \Phi_{in})$ will be $\varepsilon$-close to the energy of a continuous, piecewise differentiable field and hence larger than $\mathcal{E}(\Phi_m) - \varepsilon$. This means that, with a fine enough mesh, $\mathcal{E}(\Phi_{out}) + \mathcal{E}(\Phi_{in})$ cannot be smaller than $\mathcal{E}(\Phi_m) - \varepsilon$. On the other hand, there are discretized fields in the direct neighborhood of $\Phi_m$ whose energy cannot be larger than $\mathcal{E}(\Phi_m) + \varepsilon$. Consider now a discretized field close to the minimum, i.e. whose energy lies in the region $\mathcal{E}(\Phi_m) \pm \varepsilon$. It turns out that it cannot be much different pointwise from $\Phi_m$, because there is a continuous, piecewise differentiable field $h$-close and the collection of such fields converges to $\Phi_m$ (Step 1). It follows that the discretized pair $(\Phi_{out}, \Phi_{in})$ does indeed converge to $\Phi_m$ when the mesh gets finer. Also the total energy $\mathcal{E}(\Phi_{out}) + \mathcal{E}(\Phi_{in})$ converges to $\mathcal{E}(\Phi_m)$.

**Quadratic Convergence**

We can actually get more mileage from the estimates of Step 2. An expression for the fields over a face around the center of gravity $p_g$ is as follows (with $\delta p$ the position difference from the center):

$$\Phi_{in} = \Phi_{av} + \delta p \cdot \nabla \Phi_{in}|_{p_g} + O(h^2) \quad (5.41)$$

$$\Phi_{out} = \Phi_{av} + \delta p \cdot \nabla \Phi_{out}|_{p_g} + O(h^2) \quad (5.42)$$

and hence (in formula (5.40) and with $p_i$ appropriate positions):

$$(\Phi_{i2} - \Phi_{i1}) - (\Phi_{i2} - \Phi_{i1}) = (p_{12} - p_{22}) \cdot [\nabla \Phi_{in}|_{p_g} - \nabla \Phi_{out}|_{p_g}] + O(h^2) \quad (5.43)$$

With a mesh of size $O(h)$ we have that $p_{12} - p_{22} = O(h)$. Since also $\nabla \Phi_{out}$ and $\nabla \Phi_{in}$ converge to $\nabla \Phi_m$ in the respective regions, we have that $[\nabla \Phi_{in} - \nabla \Phi_{out}]/_{p_g}$ is $O(h)$ as well. The product is thus of $O(h^2)$.

From the theory developed in this chapter, we can, indeed, conclude that attractive models exist for a hybrid BEM/FEM method. They retain the physical properties of the original (purely capacitive, symmetrical, passive). The disturbance introduced by the interface region converges to zero one order of magnitude faster than the finite element methods themselves.

Fast quadratic convergence of the boundary field is indeed observed in practice. The experimental results we will present in the next chapter.
5.6 Conclusions

In this chapter we have discussed the convergence properties of the new hybrid element method. We have shown that the BEM and the FEM converge themselves linearly in the energy norm and that the HEM converges linearly as well. We have proven the convergence of the HEM by showing that the energy associated with the discontinuity of the field at the boundary interface contributes a negligible part to the total energy of the system, namely a part that converges to zero quadratically when the mesh gets finer.
Convergence of the HEM

We can actually get more mileage from the estimates of Step 2. An expression for the fields over a face around the center of gravity \( p \) is as follows (with \( \delta p \) the position difference from the center):

\[
\Phi_{\text{rel}} = \Phi - \delta p \cdot \nabla \Phi_{\text{rel}} + O(h)
\]

(5.41)

\[
\Phi_{\text{rel}} = \Phi - \delta p \cdot \nabla \Phi_{\text{rel}} + O(h)
\]

(5.42)

and hence (in formula (5.41) and with \( \delta p \) appropriate positions):

\[
(\Phi_1 - \Phi_2) = (\Phi - \delta p \cdot \nabla \Phi_{\text{rel}}) - (\Phi - \delta p \cdot \nabla \Phi_{\text{rel}}) + O(h)
\]

(5.43)

With a mesh of size \( \ell \), we have that \( \delta p = \ell / h \). Since also \( \nabla \Phi_{\text{rel}} \) and \( \nabla \Phi_{\text{rel}} \) converge to \( \nabla \Phi_{\text{rel}} \) in the respective regions, we have that \( \nabla \Phi_{\text{rel}} - \nabla \Phi_{\text{rel}} \|_{\|} = O(h) \) as well. The product is thus of \( O(h^2) \).

From the theory developed in this chapter, we can, indeed, conclude that attractive models exist for a hybrid BEM/FEM method. They retain the physical properties of the original (purely capacitive, symmetrical, passive) I. The distance measured by the interface region converges to zero one order of magnitude faster than the finite element methods themselves.

Fast quadratic convergence of the boundary field is indeed observed in practice. The experimental results we will present in the next chapter.


# PRACTICAL RESULTS

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## 6.1 Introduction

In chapter we consider the following main issues:

- validation of the hybrid method by comparison with other available methods such as the BEM and the FEM, when applicable;
- convergence of the hybrid method, i.e. accuracy of the method when the size of the mesh gets smaller.
The practical results, as we will see, confirm the usefulness, practicality and superiority of the hybrid method.

In this chapter we work with simple layouts, consisting of one or two conductors and the artificial “inside” region, as benchmarks. The dimensions of conductors and the “inside” region are usually in microns ($\mu m$), and the distances between them also. We work with the free space, half space and two layered media. For 2D space we work with the free space, half plane and two layered media as well. The materials we work with are vacuum with relative permittivity $\varepsilon_r = 1$ and silicon oxide ($SiO_2$) with relative permittivity $\varepsilon_r = 4$.

The accuracy of the new HEM should be validated by checking the results provided by the new method with known results. In the literature we can find many results for different benchmarks, but only some of them are confirmed by measurements. To check accuracy of the HEM we compare the results of the method with the results obtained by two different methods. We consider this comparison as sufficiently reliable.

For validation purposes we apply the hybrid modeling to benchmarks with perfect planarization. We expect the results obtained by the HEM for these cases to agree with results provided by the BEM. To make the planarization imperfect we set an appropriate dielectric permittivity in the “inside” region. For this case we expect the results of the HEM to agree with those obtained by the FEM.

We have implemented the hybrid method in two and three dimensions. For 2D hybrid modeling we have adapted the theory of the HEM to two dimensions as it is explained in Appendix 1.

We have to make a remark here. In this chapter we will focus mainly on the accuracy of the hybrid technique, not on the efficiency. We present in this chapter results of the prototype program implemented in Mathematica [Wolfram 91] which is linked to integration routines implemented in C. We are still working on improvement of the mesh generation and evaluation of integrals, which will considerably improve the time performance of the program.

### 6.2 2D validation

#### 6.2.1 Example 1

Let us consider the cross-section of one infinite line above the ground plane shown schematically in Figure 6.1. We introduce an artificial irregular domain in which we use the HEM as described earlier. The conductor has a square shape and the “inside” region has a rectangular shape. First, we assume that the “inside” region has the same permittivity as the background dielectric, $k_2 = k_1 = 1$, which corresponds to the situation when the stratification is perfect.
6.2 2D validation

Figure 6.1. The cross-section of an infinite line in a dielectric half-plane with relative permittivity $k_1$ separated from the ground plane by an “inside” region with relative permittivity $k_2$.

Table 6.1. The comparison of the ground capacitances as computed by the BEM, the HEM and the FEM for the geometry of Figure 6.1, when $k_2 = k_1 = 1$.

<table>
<thead>
<tr>
<th>$k_2$ Method</th>
<th>$N_n$</th>
<th>$n_c$</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$C_g [pF/m]$</th>
<th>$\delta [%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEM</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>26.028</td>
<td></td>
</tr>
<tr>
<td>HEM</td>
<td>8</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>26.167</td>
<td>0.567</td>
</tr>
<tr>
<td></td>
<td>16</td>
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<td>6</td>
<td>2</td>
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<td>1</td>
<td>9</td>
<td>3</td>
<td>26.051</td>
<td>0.121</td>
</tr>
<tr>
<td></td>
<td>32</td>
<td>1</td>
<td>12</td>
<td>4</td>
<td>26.030</td>
<td>0.043</td>
</tr>
<tr>
<td>FEM</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>25,911</td>
<td></td>
</tr>
</tbody>
</table>

Let us introduce parameters $n_c$, $n_x$ and $n_y$. Here, $n_c$ denotes the number of the boundary elements per edge of the conductor, $n_x$ denotes the number of the boundary elements per edge of the “inside” region in the direction of the $x$-axis, and $n_y$ in the direction of the $y$-axis. We also introduce the parameter $N_n$ which denotes the number of nodes lying on the boundary interface and $N_f$ the number of boundary elements on the boundary interface.

Let us also define the relative error $\delta$ such that:

$$\delta = \left| \frac{C_{HEM} - C_{BEM}}{C_{BEM}} \right| \times 100\% (6.1)$$

We fix the discretization on the conductor, say to 4 edges per entire conductor, and on the boundary interface. In Table 6.1 we show the results obtained for this configuration by the BEM package Space [Meijs 92], the FEM package VLSIcap [Straker 86] and by the HEM. We compare the ground capacitance $C_g$ of the conductor obtained by all packages.
Table 6.2. The convergence of the ground capacitance $C_g$ as computed by the BEM

<table>
<thead>
<tr>
<th>$n_e$</th>
<th>$C_g$ [pF/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>26.028</td>
</tr>
<tr>
<td>2</td>
<td>26.030</td>
</tr>
<tr>
<td>3</td>
<td>26.108</td>
</tr>
<tr>
<td>4</td>
<td>26.137</td>
</tr>
<tr>
<td>5</td>
<td>26.155</td>
</tr>
<tr>
<td>10</td>
<td>26.186</td>
</tr>
<tr>
<td>20</td>
<td>26.199</td>
</tr>
<tr>
<td>40</td>
<td>26.204</td>
</tr>
<tr>
<td>80</td>
<td>26.206</td>
</tr>
</tbody>
</table>

At this point we have to make few remarks. The discretization used by the HEM concerns the 1D boundary elements for the BEM and the 2D triangular finite elements for the FEM. Since the dimensions of the elements used are different it is difficult to show the convergence of the combination of the two methods at once.

In the previous chapter we have proven the linear convergence of the HEM by showing that the energy associated with the discontinuity of the field at the boundary interface converges to zero one order of magnitude faster than the BEM and the FEM themselves, with the refinement of the mesh at the boundary interface.

In our experiment we try to show this behavior in practice. We fix a certain discretization on the conductor boundary and refine the mesh on the boundary interface, while adapting the mesh in the “inside” region to the size of the mesh imposed on the boundary interface. Having a finer mesh on the conductor is not the main issue here. In Table 6.2 we show how the results for $C_g$ obtained by the BEM itself converge.

Keeping in mind the limitations of the Mathematica package, in which our prototype program has been implemented, for the size of matrices one may work with, we decided to use the most coarse discretization on the conductor as the reference.

Our expectation is that, with refinement of the boundary interface mesh, the results of the HEM will converge to the result for $C_g$ provided by the BEM for a fixed discretization on the conductor. This behavior is indeed observed. It is difficult to determine precisely the order of convergence of the HEM in this case. One may say the convergence is “nearly” linear observing the results of the HEM. The problem with “nearly” linear convergence is that in our experiment the size of the mesh used for the BEM remains the same while the mesh used by the FEM becomes finer.

The results obtained by the HEM and by the FEM package VLSIcap are not fully compatible due to different principles of work of the two methods. VLSIcap is a program which calculates interconnect and junction capacitances at the device level in very large integrated circuits. The extraction area represents the cross-section of
6.2 2D validation

The cross-section used for capacitance extraction in the VLSIcap package.

part of the layout of an integrated circuit and may consist of dielectrics, conductors and semiconductors. The Poisson equation is solved in the package by the FEM. VLSIcap reads a user’s description of the cross-section of the layout and automatically converts this description into a finite element mesh. Triangular finite elements with biquadratic basis functions are used. The initial finite element mesh is refined in order to distribute the local discretization error evenly over the extraction region. This relaxation of the mesh is performed with no influence of the user.

The user can only influence the description of the cross-section of the layout, especially the area of the cross-section, which is used by the extraction system. The FEM can be applied only to the finite, bounded area of the cross-section. The bigger this area is the more effects of the infinite electrical field can be included in capacitance modeling.

In our case the cross-section to which we apply the VLSIcap extraction package is shown in Figure 6.2.

We choose large horizontal dimension of the cross-section in comparison with the feature sizes of the conductor and the “inside” region in order to include as well as possible the effects of the fringing field.

The values of $C_g$ for the FEM are relatively less accurate because the method cannot account for the far field, but the results are nonetheless close to the results obtained by the BEM and the HEM.

Next, we assume that the “inside” region has relative permittivity $k_2 = 4$, namely we have a disturbance of the dielectric half-plane.

We validate the results obtained by the HEM for this case by comparison with results coming from the FEM package VLSIcap.
Table 6.3. The comparison of the ground capacitances as computed by the FEM and the HEM for the geometry of Figure 6.1, when \( k_2 = 4 \).

<table>
<thead>
<tr>
<th>( k_2 )</th>
<th>Method</th>
<th>( n_c )</th>
<th>( n_x )</th>
<th>( n_y )</th>
<th>( C_g ) ([\text{pF/m}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td><strong>FEM</strong></td>
<td></td>
<td></td>
<td></td>
<td>29.339</td>
</tr>
<tr>
<td></td>
<td><strong>HEM</strong></td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>31.518</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>6</td>
<td>2</td>
<td>31.417</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>9</td>
<td>3</td>
<td>31.417</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>12</td>
<td>4</td>
<td>31.373</td>
</tr>
</tbody>
</table>

The results obtained by the FEM and the HEM are displayed in Table 6.3.

Before we compare the results of the HEM obtained for homogeneous (regular) and inhomogeneous cases, let us make general estimation of changes which we expect for these cases.

We try to determine the upper bound of the changes by using the *parallel plate approximation* (we stretch the conductor so that it becomes an infinitely thin plate above the ground plane). We simplify the configuration considered in this experiment to parallel plate case shown in Figure 6.3.

The total capacitance for parallel plate case can be considered, as shown in Figure 6.3, as the series of four capacitances. When the medium is homogeneous, i.e. \( k_2 = k_1 = 1 \), the total capacitance is determined by series of four capacitances of the same value \( C_x \) (one for each 0.5\( \mu \)m) as:

\[
C_{\text{tot}} = \frac{1}{4} C_x. \quad (6.2)
\]

For the inhomogeneous medium when the permittivity \( k_2 = 4 \), the total capacitance \( C_{\text{tot}D} \) (the index \( D \) means here “disturbance”) is determined by the series of two capacitances of value \( C_x \) and two capacitances of value \( 4C_x \).

![Figure 6.3](image.png)  
*Figure 6.3.* The parallel plate configuration with four capacitors connected in series.
6.2 2D validation

Then:

\[ \frac{1}{C_{\text{tot}D}} = \frac{1}{C_x} + \frac{1}{4C_x} + \frac{1}{4C_x} + \frac{1}{C_x} = \frac{5}{2C_x}. \] (6.3)

Hence,

\[ C_{\text{tot}D} = \frac{2}{5} C_x. \] (6.4)

The relative difference between the homogeneous and inhomogeneous case which is given by:

\[ \delta = \left| \frac{C_{\text{tot}D} - C_{\text{tot}}}{C_{\text{tot}}} \right| \cdot 100\% \approx 60\% \] (6.5)

is an upper bound of the possible changes on the parallel plate approximations.

Now, returning to the hybrid modeling we notice that the change in the relative permittivity of the “inside” region causes a change in the value of the ground capacitance of about 20.5% which according to our parallel plate approximation is quite possible.
6.2.2 Example 2

The next configuration, which we will test, is similar to that from Example 1. We show the cross-section of this configuration consisting of an infinite line above the ground plane in Figure 6.4. In comparison with the previous case the width of the "inside" region is larger. Simply speaking, this means that more of the field lines will go through the "inside" region, especially the fringing field lines.

Again we compare the results obtained by the different methods when the relative permittivity of the "inside" region changes.

The results are shown in Table 6.4. The change in relative permittivity of the "inside" region causes a change in the value of the ground capacitance $C_g$ of about 26%. In comparison with the previous experiment we observe, as expected, an increase of the value of $C_g$ for $k_2 = 4$ due to the increase of the width of the "inside" region with the disturbance.
6.2 2D validation

\(C_{ij}(F.E.M., k_2 = 1)\), the value of \(C_{ij}\) obtained by the F.E.M. when \(k_2 = 1\).

Table 6.4. The comparison of the ground capacitances as computed by the BEM, the FEM and the HEM for the geometry of Figure 6.4, when \(k_2\) changes from 1 to 4.

<table>
<thead>
<tr>
<th>(k_2)</th>
<th>Method</th>
<th>(N_n)</th>
<th>(n_c)</th>
<th>(n_x)</th>
<th>(n_y)</th>
<th>(C_g[pF/m])</th>
<th>(\delta[%])</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td>26.028</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FEM</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>25.911</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HEM</td>
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<td>7</td>
<td>1</td>
<td></td>
<td>26.415</td>
<td>1.521</td>
</tr>
<tr>
<td></td>
<td></td>
<td>32</td>
<td>14</td>
<td>2</td>
<td></td>
<td>26.130</td>
<td>0.427</td>
</tr>
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<td></td>
<td></td>
<td>48</td>
<td>21</td>
<td>3</td>
<td></td>
<td>26.069</td>
<td>0.194</td>
</tr>
<tr>
<td></td>
<td></td>
<td>64</td>
<td>28</td>
<td>4</td>
<td></td>
<td>26.048</td>
<td>0.110</td>
</tr>
<tr>
<td>4</td>
<td>FEM</td>
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<td></td>
<td></td>
<td></td>
<td>31.120</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1</td>
<td>7</td>
<td>1</td>
<td></td>
<td>33.300</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>14</td>
<td>2</td>
<td></td>
<td>33.078</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>21</td>
<td>3</td>
<td></td>
<td>33.025</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>28</td>
<td>4</td>
<td></td>
<td>33.005</td>
<td></td>
</tr>
</tbody>
</table>
6.2.3 Example 3

In this example we increase the number of conductors. We consider the case of two infinite lines above the ground plane, lying above each other and separated by an “inside” region, as depicted in Figure 6.5.

![Diagram of two infinite lines with relative permittivity](image)

**Figure 6.5.** The cross-section of two infinite lines in a half-plane with relative permittivity $k_1$ separated from each other by an “inside” region with relative permittivity $k_2$.

We calculate and compare the ground capacitances of the conductors $C_{1g}$, $C_{2g}$, and the coupling capacitance $C_{12}$. We use the same strategy as in the previous examples, namely we calculate the relevant capacitances by using all packages for the different relative permittivities of the “inside” region. The results are displayed in Table 6.5.

From the results we can conclude that the change in permittivity of the “inside” region affects primarily the coupling capacitance between the conductors and also the ground capacitance of the top conductor.

We see that the change in the relative permittivity of the “inside” region $k_2$ from 1 to 4 strongly influences the coupling capacitance $C_{12}$ causing the difference of around 32% in the value of $C_{12}$.

This behavior can be verified by the FEM, which accurately models the effects of the local field.

Let us introduce the following notation:
6.2 2D validation

\[ C_{12}(FEM, k_2 = 1) \] - the value of \( C_{12} \) obtained by the FEM when \( k_2 = 1 \),

\[ C_{12}(FEM, k_2 = 4) \] - the value of \( C_{12} \) obtained by the FEM when \( k_2 = 4 \),

etc.

For the coupling capacitances calculated by the FEM and the HEM we have:

\[
\frac{C_{12}(FEM, k_2 = 4)}{C_{12}(FEM, k_2 = 1)} = 1.37, \\
\frac{C_{12}(HEM, k_2 = 4)}{C_{12}(HEM, k_2 = 1)} = 1.35.
\]

The ratios obtained for the two methods are very close and indicate a good conformance.
Table 6.5. The comparison of the ground and coupling capacitances as computed by the BEM, the FEM and the HEM for the geometry of Figure 6.5, when \(k_2\) changes from 1 to 4.

<table>
<thead>
<tr>
<th>(k_2)</th>
<th>Method</th>
<th>(n_c)</th>
<th>(n_x)</th>
<th>(n_y)</th>
<th>(C_{1g}[pF/m])</th>
<th>(\delta_{1g} [%])</th>
<th>(C_{2g}[pF/m])</th>
<th>(\delta_{2g} [%])</th>
<th>(C_{12}[pF/m])</th>
<th>(\delta_{12} [%])</th>
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<tr>
<td>1</td>
<td>BEM</td>
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<td>1</td>
<td>43.156</td>
<td></td>
<td>14.833</td>
<td></td>
<td>8.762</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FEM</td>
<td></td>
<td></td>
<td></td>
<td>44.049</td>
<td></td>
<td>14.283</td>
<td></td>
<td>9.006</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1 7 1</td>
<td>2 14 2</td>
<td>3 21 3</td>
<td>4 28 4</td>
<td>43.447</td>
<td>0.674</td>
<td>43.234</td>
<td>0.180</td>
<td>43.191</td>
</tr>
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<td></td>
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<td>45.595</td>
<td>16.291</td>
<td>45.038</td>
<td>16.928</td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>FEM</td>
<td></td>
<td></td>
<td></td>
<td>45.038</td>
<td></td>
<td>16.928</td>
<td></td>
<td>12.092</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1 7 1</td>
<td>2 14 2</td>
<td>3 21 3</td>
<td>4 28 4</td>
<td>44.863</td>
<td>0.005</td>
<td>44.824</td>
<td>0.000</td>
<td>44.824</td>
</tr>
</tbody>
</table>
6.2.4 Example 4

It can be interesting to consider the symmetric case with two infinite lines above the ground plane, lying next to each other and separated by the “inside” region, as shown in Figure 6.6. Again using all available methods, including the HEM,

![Figure 6.6](image)

**Figure 6.6.** The cross-section of two infinite lines lying next to each other in a half-plane with relative permittivity $k_1$ separated by an “inside” region with relative permittivity $k_2$.

we calculate the ground capacitances $C_{1g}$, $C_{2g}$, and the coupling capacitance $C_{12}$. We present the results obtained in Table 6.6. The discretization used in the BEM and the HEM provides the mesh of edges which is symmetric. Thus the ground capacitances of the two conductors are the same, and the value of $C_g = C_{1g} = C_{2g}$ appears only once in Table 6.6.

Analyzing the configuration investigated in this example we can expect that the disturbance region will influence the coupling capacitance between the conductors much stronger than the ground capacitances. Indeed this is observed in practice. The change in permittivity of the “inside” region causes a change in the ground capacitances of about 8.5% and in the coupling capacitance of about 33.5%.

The results of the FEM and the BEM for $C_{12}$, for when the permittivity of the “inside” region changes, are very consistent with each other. The two method provide the following ratios:

$$C_{12}(FEM, k_2 = 4) = 1.335, \quad C_{12}(FEM, k_2 = 1) = 1.334,$$

$$C_{12}(HEM, k_2 = 4) = 1.335, \quad C_{12}(HEM, k_2 = 1) = 1.334,$$

which are practically identical.
Table 6.6. The comparison of the ground and coupling capacitances as computed by the BEM, the FEM and the HEM for the geometry of Figure 6.6, when \( k_2 \) changes from 1 to 4

<table>
<thead>
<tr>
<th>( k_2 )</th>
<th>Method</th>
<th>( n_c )</th>
<th>( n_x )</th>
<th>( n_y )</th>
<th>( C_g [pF/m] )</th>
<th>( \delta_g [%] )</th>
<th>( C_{12} [pF/m] )</th>
<th>( \delta_{12} [%] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td>23.466</td>
<td>8.144</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>FEM</td>
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<td></td>
<td></td>
<td>23.151</td>
<td>8.557</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>HEM</td>
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<td>3</td>
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<td>23.701</td>
<td>1.001</td>
<td>8.243</td>
<td>1.220</td>
</tr>
<tr>
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<td>HEM</td>
<td>1</td>
<td>6</td>
<td></td>
<td>23.522</td>
<td>0.238</td>
<td>8.226</td>
<td>1.014</td>
</tr>
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<td>HEM</td>
<td>1</td>
<td>9</td>
<td></td>
<td>23.491</td>
<td>0.106</td>
<td>8.184</td>
<td>0.493</td>
</tr>
<tr>
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<td>HEM</td>
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<td></td>
<td>23.480</td>
<td>0.059</td>
<td>8.167</td>
<td>0.289</td>
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<td>0.038</td>
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<td>FEM</td>
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<td>3</td>
<td></td>
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<td>11.427</td>
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<td></td>
</tr>
<tr>
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<td>3</td>
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<td>25.631</td>
<td>10.882</td>
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<td></td>
</tr>
<tr>
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<td>HEM</td>
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<td>6</td>
<td></td>
<td>25.500</td>
<td>10.908</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>HEM</td>
<td>1</td>
<td>9</td>
<td></td>
<td>25.467</td>
<td>10.896</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>HEM</td>
<td>1</td>
<td>12</td>
<td></td>
<td>25.453</td>
<td>10.890</td>
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</tr>
<tr>
<td>1</td>
<td>HEM</td>
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<td>15</td>
<td></td>
<td>25.447</td>
<td>10.887</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Assuming that the FEM accurately treats the coupling capacitance between the conductors when the permittivity of the “inside” region changes, we can conclude that the HEM treats the capacitance \( C_{12} \) equally well as the FEM.
6.2.5 Example 5

In this section we consider a slightly more complicated structure which is shown in Figure 6.7. We see a two layered medium delimited at the bottom by the ground plane. The relative permittivity of the bottom layer is $k_1 = 4$, and the relative permittivity of the top layer is $k_2 = 1$. We place a conductor in the top layer and introduce an artificial “inside” region with relative permittivity $k_3$ in the bottom dielectric layer. We calculate the ground capacitance of the conductor by the BEM, the FEM and the HEM, and compare the results in Table 6.7.

The ground capacitance decreases with about 17.5\% when the relative permittivity $k_3$ of the “inside” region changes from 4 to 1. The parallel plate approximation (in the same manner as it has been done in the first experiment) provides an upper bound on the possible changes of about 43\%, and is confirmed by the FEM.

![Figure 6.7](image)

**Figure 6.7.** The cross-section of an infinite line in the top layer with relative permittivity $k_2$ of a two-layered medium. In the bottom layer with relative permittivity $k_1$ an “inside” region with relative permittivity $k_3$ is placed.

Table 6.7 shows a good convergence of the HEM, with respect to the BEM, for the uniform stratification of the dielectric structure. Likewise, the ratios:

$$\frac{C_{12}(FEM, k_2 = 4)}{C_{12}(FEM, k_2 = 1)} = 1.218,$$
$$\frac{C_{12}(HEM, k_2 = 4)}{C_{12}(HEM, k_2 = 1)} = 1.211,$$

show good accuracy of the HEM with respect to the FEM when a disturbance of the dielectric medium is introduced.
Table 6.7. The comparison of the ground capacitances as computed by the BEM, the FEM and the HEM for the geometry of Figure 6.7, when $k_3$ changes from 4 to 1

<table>
<thead>
<tr>
<th>$k_3$</th>
<th>Method</th>
<th>$n_c$</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$C_g [pF/m]$</th>
<th>$\delta_g [%]$</th>
</tr>
</thead>
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<tr>
<td>4</td>
<td>BEM</td>
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<td></td>
<td></td>
<td>36.201</td>
<td></td>
</tr>
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<td>FEM</td>
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<td>36.548</td>
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<td>0.146</td>
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<td>3</td>
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<td>28</td>
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<td>36.215</td>
<td>0.039</td>
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<td></td>
<td></td>
<td>29.987</td>
<td></td>
</tr>
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<td></td>
<td>1</td>
<td>14</td>
<td>2</td>
<td>29.950</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>21</td>
<td>3</td>
<td>29.911</td>
<td></td>
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<td></td>
<td></td>
<td>1</td>
<td>28</td>
<td>4</td>
<td>29.899</td>
<td></td>
</tr>
</tbody>
</table>
6.2 2D validation

6.2.6 Example 6

In this last experiment which is the most significant for 2D we consider the cross-section of two lines situated in the two-layered medium, see Figure 6.8. Conductors are placed in the different layers above each other and separated by an “inside” region which is adjacent to the dielectric interface between the two dielectric layers.

![Figure 6.8. The cross-section of two infinite lines in a two-layered medium separated by an “inside” region. The bottom layer has relative permittivity $k_1 = 4$, the top layer $k_2 = 1$ and the “inside” region $k_3$.](image)

First, we assume that the “inside” region has the same relative permittivity as the top dielectric layer $k_3 = k_2 = 1$, this corresponds to the situation when the stratification is perfect. Next, we assume that the “inside” region has the same relative permittivity as the bottom layer $k_3 = k_1 = 4$, namely we have a disturbance in the stratification. In both cases we calculate the ground capacitances of the conductors $C_{1g}$, $C_{2g}$, and the coupling capacitance $C_{12}$. The results obtained by the BEM, the FEM and the HEM for both cases are shown in Table 6.8.

As in previous experiments, we observe that the disturbance significantly influences the capacitive couplings. In this particular case the change in the permittivity of the “inside” region gives a change of about 55% in the coupling capacitance between the conductors. We also observe that the results obtained by the HEM for the ground and coupling capacitances converge well, with respect to the BEM. Furthermore, the results of the FEM and the HEM agree very well for when the permittivity of the disturbance is changed. This behavior is confirmed in practice by the ratios:

$$\frac{C_{12}(\text{FEM}, k_2 = 4)}{C_{12}(\text{FEM}, k_2 = 1)} = 1.57,$$

$$\frac{C_{12}(\text{HEM}, k_2 = 4)}{C_{12}(\text{HEM}, k_2 = 1)} = 1.56.$$
Table 6.8. The comparison of the ground capacitances as computed by the BEM, the FEM and the HEM for the geometry of Figure 6.8, when $k_3$ changes from 1 to 4

<table>
<thead>
<tr>
<th>$k_3$</th>
<th>Method</th>
<th>$n_c$</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$C_{1g}[pF/m]$</th>
<th>$\delta_{1g}[%]$</th>
<th>$C_{2g}[pF/m]$</th>
<th>$\delta_{2g}[%]$</th>
<th>$C_{12}[pF/m]$</th>
<th>$\delta_{12}[%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td>173.161</td>
<td>0.378</td>
<td>16.186</td>
<td>0.389</td>
<td>11.188</td>
<td>5.555</td>
</tr>
<tr>
<td></td>
<td>FEM</td>
<td></td>
<td></td>
<td></td>
<td>177.260</td>
<td>0.092</td>
<td>15.957</td>
<td>0.093</td>
<td>11.416</td>
<td>1.519</td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1</td>
<td>7</td>
<td>1</td>
<td>173.817</td>
<td>0.041</td>
<td>16.123</td>
<td>0.038</td>
<td>11.810</td>
<td>0.686</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>14</td>
<td>2</td>
<td>173.322</td>
<td>0.023</td>
<td>16.171</td>
<td>0.020</td>
<td>11.358</td>
<td>0.388</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>21</td>
<td>3</td>
<td>173.232</td>
<td>0.023</td>
<td>16.180</td>
<td>0.020</td>
<td>11.265</td>
<td>0.388</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>28</td>
<td>4</td>
<td>173.201</td>
<td>0.023</td>
<td>16.183</td>
<td>0.020</td>
<td>11.231</td>
<td>0.388</td>
</tr>
<tr>
<td>4</td>
<td>FEM</td>
<td>1</td>
<td>7</td>
<td>1</td>
<td>181.76</td>
<td>0.023</td>
<td>18.376</td>
<td>0.020</td>
<td>17.940</td>
<td>0.388</td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1</td>
<td>14</td>
<td>2</td>
<td>178.859</td>
<td>0.023</td>
<td>18.519</td>
<td>0.020</td>
<td>17.817</td>
<td>0.388</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>21</td>
<td>3</td>
<td>178.084</td>
<td>0.023</td>
<td>18.499</td>
<td>0.020</td>
<td>17.560</td>
<td>0.388</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>28</td>
<td>4</td>
<td>177.871</td>
<td>0.023</td>
<td>18.498</td>
<td>0.020</td>
<td>17.470</td>
<td>0.388</td>
</tr>
</tbody>
</table>
6.3 3D validation

6.3.1 Example 1

A perfectly conducting cube, with dimensions $1m \times 1m \times 1m$, in vacuum is a frequently used benchmark. We show the sketch of the situation in Figure 6.9. We introduce an artificial “inside” region in which we will use the hybrid method as explained in Chapter 4.

![Figure 6.9](image)

**Figure 6.9.** A conducting cube in a vacuum ($k_1 = 1$). An artificial “inside” region, with relative permittivity ($k_2$) and dimensions $1m \times 1m \times 1m$, is introduced.

First, we assume that the dielectric permittivity of the “inside” region is the same as the background dielectric $k_2 = k_1 = 1$. This means that there is no irregularities in the medium.

We also introduce the following parameters $n_c$, $n_x$, $n_y$ and $n_z$, which denote:

- $n_c$ - the number of triangular elements per edge of the conductor;
- $n_x$ - the number of triangular elements per edge of the “inside” region in the direction of $x$-axis;
- $n_y$ - the number of triangular elements per edge of the “inside” region in the direction of $y$-axis;
- $n_z$ - the number of triangular elements per edge of the “inside” region in the direction of $z$-axis;

The conductor is represented by a cube and the “inside” region by parallelepiped. In Figure 6.10 we show how the 2D triangular mesh over the surface of conductors...
and the “inside” region is created.

![Figure 6.10. Triangulation mesh on a cuboidal conductor. (a) \((n_x, n_y, n_z) = (1, 1, 1)\). (b) \((n_x, n_y, n_z) = (2, 2, 1)\).](image)

We introduce as well the relative error \(\delta\) such that:

\[
\delta = \left| \frac{C_{HEM} - C_{BEM}}{C_{BEM}} \right| \cdot 100\%
\]  
(6.6)

We calculate the total capacitance of the conductor. We place on the boundary of the “inside” region a uniform mesh, i.e. the size of all elements is the same. In [Ruehli 73] the author gives upper and lower bounds for the total capacitance of the conducting cube, with dimensions given in this example, as:

\[73.3\text{pF} < C < 74.3\text{pF}\]  
(6.7)

In Table 6.9 we show the results obtained by the BEM package Space [Meijs 92] and the hybrid modeling. Our reference value obtained by the BEM is out of the range given by Ruehli, but this is due to a very coarse mesh. In the case of a hybrid modeling for a fine discretization of the mesh, the size of the matrices used by the HEM gets out of hand, causing problems for our prototype program due to storage limitations.

Analyzing the results listed in Table 6.9 we observe a very good agreement of the results of the HEM with the results of the BEM and a very quick convergence, even for a quite coarse mesh on the “inside” region (while the mesh on conductor is fixed).

To investigate further the properties of the hybrid method we enlarge the “inside” region in the way shown in Figure 6.11. Even for such a configuration we observe a quick convergence of the results obtained by the HEM to the value of the total capacitance obtained by the BEM.
### Table 6.9
The comparison of the total capacitance of the conducting cube in vacuum as computed by the BEM and the HEM when $k_1 = k_2 = 1$.

<table>
<thead>
<tr>
<th>Method</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$n_z$</th>
<th>$C_y [pF]$</th>
<th>$\delta [%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td>72.169</td>
<td></td>
</tr>
<tr>
<td>HEM</td>
<td>1 '</td>
<td>1 '</td>
<td>1 '</td>
<td>72.187</td>
<td>0.025</td>
</tr>
<tr>
<td></td>
<td>1 2</td>
<td>1</td>
<td></td>
<td>72.187</td>
<td>0.025</td>
</tr>
<tr>
<td></td>
<td>1 2</td>
<td>2</td>
<td>1</td>
<td>72.180</td>
<td>0.015</td>
</tr>
<tr>
<td></td>
<td>1 2'</td>
<td>2'</td>
<td>2'</td>
<td>72.176</td>
<td>0.009</td>
</tr>
<tr>
<td></td>
<td>1 3</td>
<td>2</td>
<td>2</td>
<td>72.175</td>
<td>0.008</td>
</tr>
<tr>
<td></td>
<td>1 3</td>
<td>3</td>
<td>2</td>
<td>72.174</td>
<td>0.006</td>
</tr>
<tr>
<td></td>
<td>1 3'</td>
<td>3'</td>
<td>3'</td>
<td>72.172</td>
<td>0.004</td>
</tr>
<tr>
<td></td>
<td>1 4</td>
<td>3</td>
<td>3</td>
<td>72.172</td>
<td>0.003</td>
</tr>
<tr>
<td></td>
<td>1 4</td>
<td>4</td>
<td>3</td>
<td>72.171</td>
<td>0.002</td>
</tr>
<tr>
<td></td>
<td>1 4'</td>
<td>4'</td>
<td>4'</td>
<td>72.171</td>
<td>0.002</td>
</tr>
<tr>
<td></td>
<td>1 5</td>
<td>4</td>
<td>4</td>
<td>72.171</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>1 5</td>
<td>5</td>
<td>4</td>
<td>72.170</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>1 5'</td>
<td>5'</td>
<td>5'</td>
<td>72.170</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>1 6</td>
<td>5</td>
<td>5</td>
<td>72.170</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>1 6</td>
<td>6</td>
<td>5</td>
<td>72.170</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>1 6'</td>
<td>6'</td>
<td>6'</td>
<td>72.170</td>
<td>0.000</td>
</tr>
</tbody>
</table>

### Table 6.10
The comparison of the total capacitance of the conducting cube in vacuum (as shown in Figure 6.11) as computed by the BEM and the HEM when $k_1 = k_2 = 1$.

<table>
<thead>
<tr>
<th>Method</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$n_z$</th>
<th>$C_y [pF]$</th>
<th>$\delta [%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td>72.169</td>
<td></td>
</tr>
<tr>
<td>HEM</td>
<td>1 3*</td>
<td>3*</td>
<td>1'</td>
<td>72.335</td>
<td>0.230</td>
</tr>
<tr>
<td></td>
<td>1 6</td>
<td>6</td>
<td>1</td>
<td>72.264</td>
<td>0.131</td>
</tr>
<tr>
<td></td>
<td>1 9</td>
<td>9</td>
<td>1</td>
<td>72.249</td>
<td>0.110</td>
</tr>
<tr>
<td></td>
<td>1 6'</td>
<td>6'</td>
<td>2'</td>
<td>72.225</td>
<td>0.077</td>
</tr>
<tr>
<td></td>
<td>1 9</td>
<td>9</td>
<td>2</td>
<td>72.207</td>
<td>0.051</td>
</tr>
</tbody>
</table>
and the "inside" region is created.

We introduce a patch of material in the "inside" region that is a conducting cube in a vacuum ($k = 1$) with artificial "inside" region with relative permittivity $k_2$ and dimensions $3m \times 3m \times 1m$.

**Figure 6.11.** A conducting cube in a vacuum ($k_1 = 1$) with an artificial "inside" region with relative permittivity $k_2$ and dimensions $3m \times 3m \times 1m$. 

- Conductors
- The 'inside' region with the relative permittivity $k_2$
6.3.2 Example 2

In this experiment we deal with the configuration shown in Figure 6.12. Two conductors, having a cuboid shape, are located in a vacuum above the ground plane. They are separated by an artificial "inside" region having a parallelepiped shape and with relative permittivity \( k_2 \). When \( k_2 = k_1 = 1 \), i.e. the relative permittivity of the "inside" region is the same as the background permittivity, we are dealing with a homogeneous half-space. When \( k_2 = 4 \), we have to deal with the disturbance of the dielectric medium.

For both cases we calculate the ground capacitances and the coupling capacitance (between the conductors) by using the HEM. For a homogeneous medium we observe a good agreement between the results obtained by the HEM and the BEM. The change in the permittivity of the "inside" region causes a change in the coupling capacitance of about 30%. This behavior could have been predicted by the parallel plate approximation. In both the homogeneous and inhomogeneous cases we observe a quick convergence of the results obtained by the HEM with the refinement of the mesh.

Figure 6.12. Two conducting cubes of dimensions 1\( \mu m \times 1\mu m \times 1\mu m \) in a half-space with relative permittivity \( k_1 \), separated by an "inside" region with relative permittivity \( k_2 \).
Table 6.11. The comparison of the ground and coupling capacitances as computed by the BEM and the FEM for geometry shown in Figure 6.12, when $k_2$ changes from 1 to 4.

<table>
<thead>
<tr>
<th>$k_2$ Method</th>
<th>$n_r$</th>
<th>$n_i$</th>
<th>$C_{aF}$ (aF)</th>
<th>$b_{aF}$ (%</th>
<th>$C_{n[aF}$ (aF)</th>
<th>$b_{n[aF}$ (%</th>
<th>$S_{n[aF}$ (%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>100.065</td>
<td>0.589</td>
<td>9.623</td>
<td>0.836</td>
<td>3.252</td>
</tr>
<tr>
<td>2</td>
<td>1.6</td>
<td>1.6</td>
<td>101.111</td>
<td>0.493</td>
<td>9.936</td>
<td>0.704</td>
<td>2.617</td>
</tr>
<tr>
<td>3</td>
<td>1.8</td>
<td>1.8</td>
<td>100.655</td>
<td>0.308</td>
<td>9.832</td>
<td>0.687</td>
<td>2.617</td>
</tr>
<tr>
<td>4</td>
<td>2.0</td>
<td>2.0</td>
<td>100.559</td>
<td>0.141</td>
<td>9.704</td>
<td>0.687</td>
<td>2.617</td>
</tr>
<tr>
<td>5</td>
<td>2.2</td>
<td>2.2</td>
<td>100.373</td>
<td>0.141</td>
<td>9.704</td>
<td>0.687</td>
<td>2.617</td>
</tr>
<tr>
<td>6</td>
<td>2.4</td>
<td>2.4</td>
<td>100.206</td>
<td>0.141</td>
<td>9.704</td>
<td>0.687</td>
<td>2.617</td>
</tr>
</tbody>
</table>

Method: BEM vs. FEM
6.3 3D validation

6.3.3 Example 3

In this experiment we deal with the configuration depicted in Figure 6.13. We see two cubic conductors above the ground plane separated by an artificial “inside” region. Using the hybrid method we calculate the ground capacitances and the coupling capacitance for different permittivities of the “inside” region. For the homogeneous case, when $k_2 = k_1 = 1$, we compare the results of the HEM with the results obtained by the BEM. The general configuration of the conductors and the “inside” region is symmetrical, but once the discretization is performed the configuration of triangular faces is not symmetrical. This is the reason behind the small differences found in ground capacitances.

In Table 6.12 we display the results of this experiment. Again, we observe convergence of the results obtained by the HEM with the mesh on the boundary of the “inside” region becoming finer.

![Figure 6.13](image)

**Figure 6.13.** Two conductors lying next to each other in a half-space with relative permittivity $k_1$, separated by an “inside” region with relative permittivity $k_2$. 
Table 6.12. The comparison of the ground and coupling capacitances as computed by the BEM and the HEM for the geometry shown in Figure 6.13, when $k_2$ changes from 1 to 4.

<table>
<thead>
<tr>
<th>$k_2$</th>
<th>Method</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$n_z$</th>
<th>$C_{1g}[aF]$</th>
<th>$\delta_{1g} [%]$</th>
<th>$C_{2g}[aF]$</th>
<th>$\delta_{2g} [%]$</th>
<th>$C_{12}[aF]$</th>
<th>$\delta_{12} [%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td>79.509</td>
<td></td>
<td>79.509</td>
<td></td>
<td>3.612</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1</td>
<td>1*</td>
<td>3*</td>
<td>79.701</td>
<td>0.241</td>
<td>79.568</td>
<td>0.074</td>
<td>3.714</td>
<td>2.823</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
<td>6</td>
<td>79.723</td>
<td>0.269</td>
<td>79.568</td>
<td>0.074</td>
<td>3.698</td>
<td>2.380</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
<td>9</td>
<td>79.729</td>
<td>0.276</td>
<td>79.571</td>
<td>0.077</td>
<td>3.695</td>
<td>2.297</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>2*</td>
<td>6*</td>
<td>6*</td>
<td>79.612</td>
<td>0.129</td>
<td>79.551</td>
<td>0.052</td>
<td>3.628</td>
</tr>
<tr>
<td>4</td>
<td>HEM</td>
<td>1</td>
<td>3*</td>
<td>6*</td>
<td>9*</td>
<td>79.561</td>
<td>0.065</td>
<td>79.526</td>
<td>0.021</td>
<td>3.620</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
<td>6</td>
<td>80.627</td>
<td></td>
<td>80.406</td>
<td></td>
<td>3.760</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
<td>9</td>
<td>80.645</td>
<td></td>
<td>80.400</td>
<td></td>
<td>3.758</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
<td>9</td>
<td>80.650</td>
<td></td>
<td>80.401</td>
<td></td>
<td>3.759</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>2*</td>
<td>6*</td>
<td>6*</td>
<td>80.578</td>
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<td>3.714</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>3*</td>
<td>9*</td>
<td>9*</td>
<td>80.549</td>
<td></td>
<td>80.371</td>
<td></td>
<td>3.705</td>
</tr>
</tbody>
</table>
6.3 3D validation

6.3.4 Example 4

In this section we consider a more complicated dielectric medium. We work with the configuration illustrated in Figure 6.14. The relative permittivity of the bottom layer is $k_1 = 4$, and the relative permittivity of the top layer is $k_2 = 1$. A cuboidal conductor is lying above the “inside” region, both of which are located in the bottom layer of a two-layered dielectric medium.

![Figure 6.14](image.png)

**Figure 6.14.** A conducting cube lying in the bottom layer (with relative permittivity $k_1$) of a two-layered medium separated from the ground plane by an artificial “inside” region with relative permittivity $k_3$. 
Table 6.13. The comparison of the ground capacitance as computed by the BEM and the HEM for the geometry shown in Figure 6.14, when $k_3$ changes from 4 to 1.

<table>
<thead>
<tr>
<th>$k_3$</th>
<th>Method</th>
<th>$n_x$</th>
<th>$n_y$</th>
<th>$n_z$</th>
<th>$C_g [\mu F]$</th>
<th>$\delta [%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>BEM</td>
<td>1</td>
<td></td>
<td></td>
<td>295.788</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HEM</td>
<td>1 3*</td>
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6.4 Conclusions

In this chapter we have tested the hybrid element method for basic benchmarks in both two and three dimensions. The hybrid method handles well the disturbance in (the stratification of) the dielectric layers. This has been confirmed especially in the 2D cases, when the local behavior of the electric field could be validated by the FEM. In the 3D cases, we have to rely on the parallel-plate approximation as an indication for the change in capacitance due to disturbances.

In both the 2D and 3D cases we have observed a good convergence of the HEM, with respect to the BEM, for perfect uniformly stratified media. We have also applied the HEM for non-uniformly stratified media.

The disturbance in the stratification of the dielectric interface or simply the disturbance of the dielectric medium can not be covered by the BEM itself without major complications. The FEM, in turn is too costly for analyzing the entire 3D dielectric structure of more complicated circuits. The hybrid method, taking advantage of the strong points of both the BEM and the FEM, seems to be a good tool to verify the influence of irregularities in the stratification of the dielectric structure on the capacitances.
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Chapter 7

OTHER APPLICATIONS OF THE HEM

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7.1 Introduction

In this chapter we will discuss the possible extensions and the application to other domains of the hybrid element method.

As we see it, the HEM can be applied to the following problems:

- **non-conformal meshes** at the boundary interface between the “outside” and “inside” regions;
- **RC modeling**, namely to combine the resistance network, obtained by the FEM, with the global capacitance network, obtained by the BEM, by means of transformers;
- **device modeling**, i.e. to combine detailed device models, obtained by the FEM or other similar methods, with the global capacitances, obtained by the BEM, again by using transformer concept.

In the subsequent sections we discuss each of the eventual applications at least in principle.
7.2 Non-conformal meshes

In the current state of the hybrid method we assume that the 3D finite element mesh coincides with the 2D boundary element mesh. Theory states that both the BEM and the FEM converge linearly in the energy norm. The convergence of both methods depends on the types of elements and the types of approximations which are used. Often it may happen that we will be satisfied with the results of the BEM for a rather coarse mesh while we want to have more accurate model for the FEM, i.e. finer 3D mesh for the FE region. This problem is illustrated in Figure 7.1. Two overlapping non-conformal triangulation meshes are shown. The coarse mesh represents the “outside” boundary mesh, the fine mesh represents the “inside” finite element mesh.

From the outside we have for each triangular element:

- the charge $\sigma_i$, associated with $i^{th}$ face;
- the Galerkin average potential $\phi_i$,

as used by the BEM.

Let us assume that in the same way we can assign the face charges and the face potentials to the triangular elements in the finer inside mesh. We distinguish the face charges and potentials for the “inside” triangular elements by the superscript “F”.

For the faces on the interface boundary from inside, the node charges and the node potentials, which are used by the FEM, are denoted by $\delta_i$ and $\phi_i$, respectively.

We know how to construct the outside capacitive model for the coarse outside mesh associated with $\sigma_i$’s and $\phi_i$’s by using the BEM. We also know how to calculate the capacitance model in the “inside” region. The inside model relates $\delta_i$’s to $\phi_i$’s. One may say that the outside capacitive model is element-wise since it works with $\sigma_i$’s and $\phi_i$’s assigned to elements, while the inside capacitance model can be called node-wise since it works with nodal values of $\delta_i$ and $\phi_i$.

Matching of the capacitive element-wise model with the capacitive node-wise model can be done in two steps as follows:

1. matching of the face potentials and face charges between the coarse outside and fine inside meshes by using the transformer concept;
2. matching of the face potentials and the face charges with the node potentials and the node charges on the fine inside mesh by the transformers as described in Chapter 4.
7.2 Non-conformal meshes

Figure 7.1. Two non-conformal meshes at the boundary interface. Thick lines represent the outside coarse mesh, fine lines represent the inside fine mesh. The centers of gravity of the elements from the outside are denoted by black circles, those from the inside by black squares.

Let us focus first on step 1. We want to use the transformer concept in step 1, since the transformer is a good model, i.e. non-dynamic, lossless and reciprocal.

To explain how the concept of a generalized transformer can be applied in this situation, let us consider the boundary mesh at the interface, shown in Figure 7.2.

Let us take the first triangle in the “inside” mesh. This triangle can be split into three parts depending on the intersections with the triangles from the “outside” mesh, as:

\[ S_1^F = S_{1i}^F + S_{1k}^F + S_{1h}^F \]  

(7.1)
Other applications of the HEM

7.2. Non-penetrating interfaces

In the present section we show how a charge or potential may penetrate through each other to achieve a charge or potential that is equal in value and opposite in sign on each side of the boundary interface. This is done by the hybrid edge method (HEM). Let us consider a problem involving two overlapping tetrahedrons. The overlapping regions are to be treated as single elements in the two meshes. From the outside we have for each triangular charge or potential:  

**Figure 7.2.** Partitioning of the first triangle in the “inside” mesh into three parts depending on the intersection with triangles in the “outside” mesh.

Referring to Figure 7.2 we distribute the “outside” charge $\sigma_i$ evenly over the elements from the “inside” mesh. This means that the charge $\sigma_i$ will contribute to the charge $\sigma^F_j$ proportionally to the common area of the $i^{th}$ triangle from outside with the $j^{th}$ triangle from inside. For the case shown in Figure 7.2 we have:

$$\sigma^F_i = \frac{S_{il}^F}{S_i^l}\sigma_1 + \frac{S_{1i}^F}{S_i}\sigma_i + \frac{S_{ik}^F}{S_k}\sigma_k.$$  (7.2)

We apply a similar trick to the potentials. We write the potential $\Phi_i$ as the weighted sum of the potentials $\Phi^F_j$ of elements from the inside, which pertain to the $i^{th}$ outside face. For the case shown in Figure 7.3 this can be written as:

$$\Phi_i = \frac{S_{il}^F}{S_i^l}\Phi^F_1 + \frac{S_{1i}^F}{S_i}\Phi^F_2 + \ldots + \frac{S_{ik}^F}{S_k}\Phi^F_k.$$  (7.3)

Globally the charge and potential distribution is given by:

$$\sigma^F_b = T_F\sigma_b,$$  (7.4)

$$\Phi_b = T^F_F\Phi^F_b,$$  (7.5)

here the index “b” means the boundary interface and

- $\sigma_b$ is the vector of element charges on the “outside” mesh at the boundary interface;
- $\sigma^F_b$ is the vector of element charges on the “inside” mesh at the boundary interface;
- $\Phi_b$ is the vector of face potentials on the “outside” mesh at the boundary interface;
- $\Phi^F_b$ is the vector of face potentials on the “inside” mesh at the boundary interface,
7.2 Non-conformal meshes

Figure 7.3. Specifying the contributions to the potential in the $i^{th}$ node of the “outside” mesh at the boundary interface coming from the elements in the “inside” mesh.

and $T_F$ the transformer matrix is such that:

$$T_{Fij} = \begin{cases} \frac{s^F_{il}}{3j} & \text{if the } i^{th} \text{ face from the “inside” mesh lies partially inside the } j^{th} \text{ face from the “outside” mesh;} \\ 0 & \text{otherwise, i.e. when } i^{th} \text{ face from inside doesn’t overlap with the } j^{th} \text{ face from outside.} \end{cases}$$ (7.6)

In the second step of constructing of the hybrid model we have to match the face potentials $\Phi^F_i$’s and the face charges $\sigma^F_i$’s with the node potentials $\Phi^F_j$’s and the node charges $\delta_h$’s. We do this the in the same way as has been described in Chapter 4. Let us consider the triangulation mesh of the fine “inside” mesh of the interface boundary shown in Figure 7.4.

For each face from outside of this fine mesh we have an average potential $\Phi^F_i$ over the $i^{th}$ face and a constant charge $\sigma^F_i$. From inside for each node in the mesh we have a node potential $\phi_\alpha$ associated with the node $\alpha$ and an overall node charge. According to the theory presented in Chapter 4 the distribution of charges and potentials can be described by using the transformer matrix $T$, as:

$$\delta_h = T \sigma^F_h,$$ (7.7)

$$\Phi^F_i = T^T \phi_\alpha.$$ (7.8)

with the transformer matrix $T$ defined as:

$$T_{ij} = \begin{cases} \frac{1}{3} & \text{if the } i^{th} \text{ node belongs to the } j^{th} \text{ face of the fine mesh on the boundary interface;} \\ 0 & \text{otherwise.} \end{cases}$$ (7.9)
Other applications of the HEM

Figure 7.4. The triangulation of the “inside” mesh at the boundary interface. The face and node charges and potentials are shown.

Assuming that the model of this part of the boundary interface is correct, the final global model consists of capacitive models from the “inside” and “outside” regions, obtained by the FEM and the BEM respectively, and combined by a cascade of transformers, as illustrated in Figure 7.5.

Figure 7.5. The block structure of the network with a cascade of transformers.

To calculate the final purely capacitive model we have to combine:

- the “inside” model described by:

\[
\delta_b^F = H \phi_b^F; \tag{7.10}
\]
7.3 RC modeling

- the "outside" model described by:

\[
\begin{bmatrix}
C_{cc} & C_{cb} \\
C_{Tcb} & C_{bb}
\end{bmatrix}
\begin{bmatrix}
\Phi_c \\
\Phi_b
\end{bmatrix} =
\begin{bmatrix}
\sigma_c \\
-\sigma_b
\end{bmatrix},
\]

(7.11)

- the first cascade of transformers described by:

\[
\sigma_b^F = T_F \sigma_b,
\]

(7.12)

\[
\Phi_b = T_F^T \Phi_b^F;
\]

(7.13)

- the second cascade of transformers described by:

\[
\delta_b^F = T \sigma_b^F,
\]

(7.14)

\[
\Phi_b^F = T^T \phi_b^F.
\]

(7.15)

Eliminating all parameters associated with the boundary interface and introducing \(T_{tot} = TT_F\), we obtain:

\[
\sigma_c = \left[ C_{cc} - C_{cb} T_{tot}^T (T_{tot} C_{bb} T_{tot}^T + H)^{-1} T_{tot} C_{cb}^T \right] \Phi_c = C \Phi_c,
\]

(7.16)

Using the incidence matrix \(A\) one can easily find the short-circuit capacitance matrix:

\[
C_s = A^T C A
\]

(7.17)

To avoid all the multiplications of the transformer matrices one may attempt to combine the cascade of transformers into one transformer \(T_{tot}\). The entries \([T_{tot}]_{kj}\) of the new transformer, created by joining the cascade of transformers, are defined as:

\[
[T_{tot}]_{kj} = \begin{cases} 
\frac{1}{3} \frac{S_k^F}{S_j} & \text{if the } k^{th} \text{ node belongs to the } i^{th} \text{ face from the } \text{"inside" mesh which lies partially inside the } j^{th} \text{ face from the } \text{"outside" mesh on the boundary;} \\
0 & \text{otherwise.}
\end{cases}
\]

(7.18)

7.3 RC modeling

If one neglects any inductive effects, the behavior of IC interconnects can be validated by simulation of an equivalent RC model. Practical experiments have proved that the distributed RC effects for IC interconnects can be modeled accurately by subdividing the interconnects into small elements and replacing them by a lumped
RC model. For each element, the total capacitance $C$ is divided over the nodes of the lumped resistive model represented by a total resistance $R$. The distribution of total resistances and capacitances can be done in many ways, as it has been described in [Su 86], [Genderen 88], [Harbour 88], [Harbour 89].

All these techniques first construct an RC network, which models the distributed resistances and capacitances, and then perform a network reduction on it, which provides a network with a smaller number of nodes but still behaving (approximately) the same as the original network.

Here we focus on the construction of an RC network. Examples of how to construct an initial RC network can be found in [Genderen 88], [Harbour 88], [Harbour 89].

The resistive network is obtained by the FEM. The global capacitances are obtained by the BEM. In order to construct an initial RC network, the capacitances should be uniformly distributed over the finite element mesh. In the global capacitance model we work with ground capacitances and coupling capacitances. For a triangular element, the total ground capacitance $C'$ associated with this element is divided into three equal ground capacitances connected to the three nodes of the equivalent resistance network of this element. This procedure is shown in Figure 7.6(a). By analogy in the 1D case the ground capacitance associated with the edge is distributed evenly between the two nodes, as shown in Figure 7.6(b). For the coupling capacitances the distribution shown in Figure 7.7 has been used. The capacitance distribution presented here is rather intuitive and based on practical experiments.

We propose as an alternative to use the hybrid method for RC modeling. The main idea behind this approach is to use 3D FEM inside the conductors and the global capacitance modeling by using the BEM on the surface of the conductors. The interface between the capacitive and resistive models would be given by an ideal transformer as described in Chapter 4.

Then if we consider two tetrahedral finite elements representing the conductors we obtain two models: a node-wise resistive and an element-wise capacitive, as shown in Figure 7.8.

We propose to introduce transformers on the triangular boundary faces of the conductors and to combine them with the capacitance network obtained by the BEM. Subsequent elimination of the transformers, according to the methodology presented in Chapter 4, yields a node-wise capacitance network spanned on the conductor mesh. This new capacitance network can be combined with the resistance network in the nodes of the conductor mesh, as is illustrated in Figure 7.9.

The new circuit model preserves the properties of the original. It is non-dynamic, lossless and passive.
Figure 7.6. Construction of the RC network. Distribution of the ground capacitances in (a) 2D triangular element, (b) 1D edge element.
Figure 7.7. Construction of the RC model for two triangular finite elements. Distribution of the coupling capacitances in: (a) 2D, (b) 1D.
Figure 7.8. Part of the network obtained from the resistance and the capacitance extraction independently. For the sake of clarity, we do not show all the capacitive couplings.

Figure 7.9. Part of the network obtained by the hybrid modeling after elimination of transformers. For the sake of clarity, we do not show all coupling and ground capacitances.
Device modeling

Device modeling is not the main topic of this thesis, yet we give a few ideas about how our method can be applied to it. The hybrid element method for capacitance extraction and its extension to the RC modeling problems allow us to handle structures such as diffused resistors, poly resistors and gate oxide capacitors. The cross-sections of these are shown in Figure 7.10.

In the case of a diffused resistor we have to deal with nonlinear effects, since the thickness of the diffusion region depends on the applied voltage. To overcome repetitions for each different bias or dealing with the Poisson equation, we perform only once a calculation of the “diffusion” capacitance and use certain formulas to predict its value for different applied voltages.

Until now we have assumed that the silicon substrate is a perfect conductor. This assumption is valid only when the substrate is heavily doped. But when the bulk dopant concentration is low, the effective capacitance between the metal and the ground plane is a function of the potential applied to the metalized interconnect. The semiconductor under the interconnect may become depleted depending on the applied potential. As a result, the capacitance between the metal and the ground plane becomes a function of the metal bias and the signal voltage. Then we must solve the modeling problem of the (non-linear) Poisson equation.

It should also be possible, by means of the hybrid method, to combine the device models with the global capacitance model. Then the active devices, such as MOS transistors for example, can be enclosed in “inside” regions in which special transistor effects can be modeled by using the FEM. In the “outside” region the global capacitive modeling is performed. A sketch of the situation is shown in Figure 7.11. The two models, obtained by the FEM and the BEM, are connected by a transformer interface as described before. This hybrid approach can be applied to a variety of semiconductor devices.
Figure 7.10. The cross-sections of: (a) diffused resistor, (b) gate oxide capacitor, (c) poly resistor.
7.4 Device modeling

Device modeling is not the main topic of this thesis, yet we give a few ideas about how our method can be applied to it. The hybrid element method for capacitance extraction and its extension to the FE model solving problems allow us to handle structures such as different layers and two-conductor circuits. The capacitances of these are shown in Figure 7.11.

The case of a diffused resistor we have to deal with nonlinear effects, since the thickness of the diffused region depends on the applied voltage. To overcome approximations for such different data or dealing with the Poisson equation, we perform only once a calculation of the diffusion capacitance and use certain formulas to predict its value for different applied voltages.

Until now we have assumed that the silicon substrate is a perfect conductor. This assumption is valid if the thickness is beyond defined. But when the bulk doping concentration is beyond defined, the metal and the ground plane is a non-conductor, and the substrate is connected to the external interconnect.

The semiconductor interconnects, to some extent, depend on the applied potential. The metal and the ground plane becomes a non-conductor, and the silicon substrate becomes a conductor, as shown in Figure 7.11. Then we must solve the modeling problem.

It should also be possible, by using the hybrid method to combine the device models with the global capacitance model. Then the active devices, such as MOS transistors for example, can be enclosed by “mode” regions in which special transmission effects can be included. The final result is shown in Figure 7.11.

The two models, obtained by the FE-M and the HEM, are connected by a transformer interface, as illustrated in Figure 7.11. This hybrid approach can be applied to a number of cases.

Figure 7.11. The cross-section of a complex dielectric medium. The dashed lines mark the fictitious boundaries of the “inside” region in which the transistor is enclosed.
Bibliography


8.1 Introduction

In this chapter we discuss how the theoretical concepts of the hybrid modeling for capacitance extraction can be implemented in a practical and efficient extraction program.

In this chapter we will often refer to the extraction system Space [Meija 88], [Meija 97]. This extraction system is an integral part of the Netlist VLSI design system [Dewide 86], which contains the framework and tools allowing the design and verification of integrated circuits. Space is used for the verification of the design layout. It constructs an equivalent electrical circuit representation of the layout. Space is capable of performing 3D capacitance extraction, resistance extraction, RC extraction. It also simulates MOS and bipolar devices and takes into account the effects connected with these devices. As a result, an equivalent
Figure 7.11. The cross-section of a complex dielectric medium. The dashed lines mark the fictitious boundaries of the “inside” region in which the transient is enclosed.
Chapter 8

IMPLEMENTATION OF THE HEM IN THE EXTRACTION SYSTEM

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8.1 Introduction

In this chapter we discuss how the theoretical concept of the hybrid modeling for capacitance extraction can be implemented in a practical and efficient extraction program.

In this chapter we will often refer to the extraction system Space [Meijs 88], [Meijs 92]. This extraction system is an integral part of the Nelsis VLSI design system [Dewilde 86], which contains the framework and tools allowing the design and verification of integrated circuits. Space is used for the verification of the design layout. It constructs an equivalent electrical circuit representation of the layout. Space is capable of performing 3D capacitance extraction, resistance extraction, RC extraction. It also recognizes MOS and bipolar devices and takes into account the effects connected with these devices. As a result, an equivalent
electrical model is obtained, which can be simulated by different types of simulators in order to check the correctness and the performance of the designed circuit. If the design circuit does not satisfy the requirements, the layout can be modified and verified again, until the requirements are met. This step in the design loop allows to avoid verification of the design by very costly fabrication of the designed circuit.

Space is an accurate and efficient extraction system, which uses a scanline technique. All extraction operations are performed on the fly in one pass over the layout. We will discuss this technique in more detail, since it is an essential part of the extraction system.

We will also discuss how the hybrid modeling can be integrated in the frame of the Space extractor, and the problems connected with it, such as the 3D mesh generation. But first we discuss the prototype implementation of the hybrid method for the capacitance extraction.

8.2 Prototype implementation

For validation and testing purposes we have developed a stand-alone extraction package linked to Mathematica [Wolfram 91] for user input and visualization purposes.

The algorithm used can be briefly described in the following steps [Nowacka 96]:

1. The data, consisting of the description of the geometry and physical properties of the structure of IC, is read in. The data contains the location, dimensions and requested refinement of the conductors and the “inside” region, and the configuration of the dielectric layers.

2. According to the input data, a mesh is generated automatically. A 2D boundary mesh on the surface of the conductors and a 3D mesh for the “inside” region. At the places where the two meshes meet at the boundary interface, they must coincide.

We restrain ourselves to orthogonal layouts only. Conductors and the artificial “inside” regions are parallelepipeds.

To generate the 2D mesh on the conductors, the surfaces of the conductors are divided into rectangles and then each rectangle is divided into two triangles.

To generate the 3D mesh, consisting of tetrahedrons, the parallelepiped representing the “inside” region is divided into smaller parallelepipeds and then each of these is partitioned into six tetrahedrons. The subdivision into tetrahedrons is done in such a way that the edges on the contour of the small parallelepipeds coincide with each other.
3. The capacitance matrix $H$ for the “inside” region is calculated.

To calculate efficiently the capacitance matrix resulting from the FEM we use the so-called frontal solution scheme.

The frontal solution method has been successfully used in two dimensions. It assumes, in the 2D case, that a line-shaped front sweeps over the finite element mesh and the contribution of each element is added to the intermediate capacitance matrix, called the frontal matrix, as the front-line passes the element.

Of course this approach can be extended to three dimensions. The front-line changes into the front-plane and we pass with the front-plane over the elements of the 3D mesh. Within the front-plane we have to choose an algorithm for scanning the cross-section of the 3D mesh, which then is two dimensional. The method of local scanning of a 2D cross-section, i.e. the way the elements in the cross-section would be sorted, must be decided by the designer of the software.

To illustrate how the frontal method works in three dimensions we consider the mesh that consists of the cuboids which are partitioned into six tetrahedrons each. Taking as an example the cube shown in Figure 8.1(a), the tetrahedrons are contributing to the capacitance matrix in the following sequence of quadruples of nodes: \{1, 2, 3, 4\}, \{2, 3, 4, 5\}, \{2, 4, 5, 6\}, \{3, 4, 5, 7\}, \{4, 5, 6, 7\}, \{5, 6, 7, 8\}. The front-plane sweeps over the cube from the left to the right, visiting the elements in the sequence of their appearance. The contribution of the capacitances of the elements are successively added to the intermediate capacitance matrix as is shown in Figure 8.1(b).

Usually we deal with a more complex mesh of the finite elements which contains many internal nodes. Let us consider a part of some hypothetical 3D mesh as we show this in Figure 8.2.

When the front-plane has passed over all the elements connected to an internal node, all the non-zero entries in the row and column corresponding to this node are known, and the node is ready to be eliminated. In the matrix representation this means that the row and column assigned to the node can be eliminated from the capacitance matrix in order to reduce the memory required for storing of the matrix. We repeat this process until all the elements have been swept by the front-plane and all internal nodes of the mesh have been eliminated.

For clarity, Figure 8.2 shows a mesh constructed of cubes. We assume that each cube is partitioned in six tetrahedrons. It is easy to see that nodes $i$ and $j$ can be eliminated when the front-plane reaches position $A_3$ and nodes $k$ and $l$ can be eliminated when the front-plane is at the position $A_4$.

For much finer meshes the frontal solution scheme results in a significant reduction of the memory usage in comparison to the case where the solution is
denotes non-zero elements of the intermediate capacitance matrix

Figure 8.1. (a) Decomposition of a cube into six tetrahedrons. (b) Successive contribution of the tetrahedrons into the intermediate capacitance matrix. We show only the upper triangular part of the capacitance matrix since it is symmetric.
8.2 Prototype implementation

Figure 8.2. An example of a more complex mesh with many internal nodes, obtained by reduction of the internal nodes after the entire capacitance matrix is completed.

4. The calculation of the relevant capacitance matrix for the "outside" region is done in the following steps:

(a) Calculation of the elastance matrix $G$ (see Equation (2.5)). This step covers the numerical evaluation of the Green's function integral when the integrand doesn't contain singularities. The singular or nearly singular integration is performed analytically.

(b) Calculation of the matrix $G^{(n)}$ (see Equation (2.4)). This step covers the numerical evaluation of the integral of the normal derivative of the Green's function. We will use analytical integration for nearly singular integrands.

(c) Calculation of the capacitance matrix $C$, which describes the capacitance connection between each pair of boundary elements (including the capacitances to the ground plane).

To obtain the capacitance matrix for the "outside" region we work with full matrices and the exact inverse of the $G$ matrix.

5. The successive introduction and elimination of the transformers takes place, as has been explained before. We repeat this process for each boundary face lying on the boundary interface between two regions.

6. Once the "reduced" capacitance matrix for the "outside" model is obtained, we combine the "outside" and the "inside" models. This step consists of
adding the entries of the matrix $H$ to the relevant entries of the “reduced” capacitance matrix for the “outside” region.

7. The Gaussian elimination of the boundary nodes on the boundary interface is done, which provides the capacitance matrix for all pairs of boundary faces lying on conductors only.

8. The calculation of the short circuit capacitance matrix $C_s$ is done.

In the next section we give an indication of how the hybrid modeling can be implemented in the layout-to-circuit extraction system.

### 8.3 Practical implementation in the extraction system

We are currently working on implementing the hybrid method, as described above, in our VLSI layout verification package Space. One of the main facilities provided by Space is the 3D capacitance extraction based on the BEM. Space reads the layout and technology databases and defines a window which sweeps over the layout. In each position of the window, the 2D mesh on the conductors is generated and the Green’s function integral for all pairs of the boundary elements is evaluated within the window. Moving the window about half of the window size, Space calculates again the relevant integrals. In such a way the elastance matrix is only partially specified and can be inverted on the fly by using the so-called Schur algorithm which calculates the approximate (maximum-entropy) inverse. More details about the Schur algorithm can be found in [Dewilde 88], [Nelis 89], [Dewilde 90], [Meijs 92].

In the case of the hybrid method the calculation of the inverse of the elastance matrix remains the same. But the calculation of the “outside” model within the window must be completed by including the contribution of the integral of the normal derivative of the Green’s function. New in the implementation of the hybrid method is the tackling of the disturbance region, i.e. the 3D mesh generation and the calculation of the relevant capacitance model. The next point of focus for the implementation of the hybrid method is to introduce and eliminate the transformers. This can be done on the fly as it is done in our prototype program which we presented above.

#### 8.3.1 The scanline technique for capacitance extraction

Scanline algorithms have proven to be efficient for geometric problems in VLSI CAD such as design-rule checking and layout-to-circuit extraction as done by Space. They solve efficiently many geometrical and topological problems, such as detection, reporting and processing of intersections. The scanline is here understood as a straight vertical line which sweeps over the layout of integrated circuit.
8.3 Practical implementation in the extraction system

During the sweep operation, the scanline encounters the input line segments. At each position of the scanline a cross-section of the layout along the scanline is maintained and layout-to-circuit extractor performs necessary calculations in order to obtain an equivalent electrical model.

The scanline-based implementation of the capacitance modeling in a layout-to-circuit extraction program is schematically shown in Figure 8.3. For clarity of the picture, we show only the view from the top on the three conductors, but the capacitive coupling is also between boundary elements on the top, bottom and the sides of the conductors positioned within the window.

![Figure 8.3](image)

**Figure 8.3.** (a) An example of three conducting lines in 3D space. (b) The view from the top on the conducting lines. The coupling capacitances within the window are shown.

The input for the extraction process consists of a geometrical description of a given layout of an integrated circuit in the form of a sorted edge description of the contours. The scanline sweeps the layout of a circuit, say from left to right.
However, not all couplings need to be calculated within an entire layout of the integrated circuit. The most significant coupling effects are for elements within a certain distance from each other. For this reason the scanline technique for capacitance extraction has been enriched by the “windowing” method.

For a layout of given height $H$ and width $W$, $d$ is the distance over which coupling capacitances are considered significant. The algorithm defines a window of width $2d$ and height $H$ which is swept along the scanline, as shown in Figure 8.4, with discrete steps of half of the window size, namely $d$.

![Figure 8.4. Sweeping of the window over the layout along the scanline.](image)

At each position of the scanline, the conductors are recognized from a combination of different mask layers and the 2D boundary element mesh is generated on conductors within the window. The boundary elements within the window are coupled with each other. Thus the Green’s function must be evaluated for all pairs of coupled boundary elements and the elastance matrix is inverted on the fly by using the so-called Schur algorithm. The result of the approximate inversion is the capacitance coupling within the window at given position. To explain how the capacitance matrix related to the entire chip layout can be constructed let us consider the following example. We take a layout which can be partitioned in three strips denoted here as $S_1$, $S_2$, and $S_3$, of width $d$ each. We scan the layout with the window of the width $2d$. The scheme to calculate the capacitance matrix of the entire layout is illustrated in Figure 8.5.

In Figure 8.5 $C(1, 2)$ denotes the capacitance matrix in the strip $(S_1 \cup S_2)$, $C(2, 3)$ denotes the capacitance matrix in the strip $(S_2 \cup S_3)$ and $C(2, 2)$ the capacitance matrix in the strip $S_2$. For two positions of the window associated with the scanline we have the capacitance matrices $C(1, 2)$ and $C(2, 3)$. Both matrices contain the contributions of the capacitive couplings within the strip $S_2$. To avoid a double
8.3 Practical implementation in the extraction system

\[
\begin{bmatrix}
C
\end{bmatrix} = \begin{bmatrix}
C(1, 2)
\end{bmatrix} + \begin{bmatrix}
C(2, 3)
\end{bmatrix} - \begin{bmatrix}
C(2, 2)
\end{bmatrix}
\]

**Figure 8.5.** A single step in the construction using the hierarchical Schur algorithm.

appearance of the common capacitive coupling in the final capacitance matrix the contribution of \(C(2, 2)\) must be subtracted. Proof of the correctness of the method and its validation is given in [Nelis 89], [Meijs 92].

Analogous techniques can be used for larger layouts, this is illustrated in Figure 8.6, showing the typical banded structure of the resulting capacitance matrix.

\[
\begin{array}{|c|c|c|c|c|}
\hline
S_1 & S_2 & S_3 & S_4 & S_5 \\
\hline
\end{array}
\quad
\begin{array}{|c|c|c|c|c|}
\hline
S_1 & S_2 & S_3 & S_4 & S_5 \\
\hline
\end{array}
\]

**Figure 8.6.** Construction of the capacitance matrix for a larger layout, divided in five strips.

From such an element-wise capacitance matrix the multiconductor capacitances must be derived. This is done by determining the multi-conductor short-circuit capacitance matrix \(C_s\) given by:

\[
C_s = A^TCA,
\]

(8.1)

where \(A\) is an incidence matrix as given in Equation (2.65), and is sparse. Thus to obtain the \(C_s\) matrix we do not need to perform full multiplication of the matrices as given by (8.1), but one may use the following algorithm to determine the ground and coupling capacitances for conductors \(I\) and \(J\):
if $i = j$  # diagonal entry
    \( C_I := C_I + C_{ij} \)
else if \( I = J \)  # nodes are on the same conductor
    \( C_I := C_I + 2C_{ij} \)
else  # nodes are on different conductors
    \( C_I := C_I + C_{ij} \)
    \( C_J := C_J + C_{ij} \)
    \( C_{IJ} := C_{IJ} - C_{ij} \)

8.3.2 Algorithm for hybrid modeling in Space

In this section, we discuss how the hybrid method presented in Chapter 4 can be implemented in the Space package.

The method we propose consists of the following steps:

1. **Prescan Layout** Search for imperfect planarization. Determine the location and size of disturbances in the stratification.

   Make a contour edge description of the “inside” region and add this description to the original layout description of an integrated circuit.

2. **Scan Layout** Screen a given layout from left to right with a window of width $2d$ and a step size of scanning $d$. As the result, subsequent windows will overlap each other by half of their width.

   For each window of width $2d$ and for each overlap of the windows of width $d$, perform the subsequent steps 3 to 9.

3. **Generate Mesh** Generate a triangular boundary element mesh on the conductors and boundaries of the “inside” regions, with special constraints for the size and shape of elements.

   Generate from a given triangulation mesh on the contour of the “inside” region, the 3D mesh consisting of tetrahedrons. Use the modified advancing front method. Take care of the connectivity of conductors and regions of disturbances, namely the meshes must coincide with each other.

4. **Calculate Capacitances in the “Outside” Region** For each pair of boundary elements in the current window calculate the mutual capacitances, including capacitances to the ground.

5. **Introduce and Eliminate Transformers** Introduce transformers for the elements at the boundary interface and eliminate them as has been explained in Chapter 4.

6. **Calculate Capacitances in the “Inside” Region** For each 3D finite element calculate an equivalent capacitive model with capacitances along edges of the element. Assemble the capacitive models of the elements.
7. **Join Circuits** Combine the modified, due to transformers, outside model with the inside model by adding the relevant capacitance values, as explained in Chapter 4. Calculate the short-circuit capacitance matrix by elimination of the nodes at the boundary interface.

8. **Update Circuit** Derive the lumped, two-terminal, capacitances from the short-circuit capacitance matrix.

9. **Clean Up** Move the window about a distance $d$ to the right to the new position, forgetting the layout to the left of the current window.

### 8.4 3D mesh generation

#### 8.4.1 Introduction

In this section we study the problem of *mesh generation*. As we have mentioned before, for the purpose of hybrid modeling the 2D triangulation mesh must be created on the surface of conductors and the 3D tetrahedrization mesh in the so-called "inside" region. A special care must be taken concerning the connectivity of the conductors and eventual "inside" regions. We search for methods of mesh generation using 2D and 3D finite elements which would automatically derive the 2D and 3D meshes from a given layout description of an integrated circuit.

Until now, process simulators have been used to determine, via simulation, the geometry of the structures of IC's. However, process simulators are not free of disadvantages such as:

- a detailed description of the processing steps must be available;
- the process simulator provides far too much information than needed for solving the capacitance modeling problem.

Thus we have to develop a technique which produces a geometric model of the finished IC. The modeling method should take care of placing of conductors and connected with this eventual disturbances in stratification of the dielectric structure of an IC.

Once the model of the layout of an IC is obtained one may attempt to generate the desired meshes. In hybrid modeling for a regularly stratified part of an IC a 2D triangulation mesh must be generated on the surface of conductors. In our extraction package *Space* the 2D mesh generation has been successfully implemented. *Space*, from a given geometrical description of the layout, generates a regular triangulation on the conductors. The regularity of the mesh is a desired feature, since it improves the numerical accuracy of the BEM. In order to obtain regular mesh certain constraints must be forced upon the area, length of edges and internal angles of
element in the mesh. Space, depending on the measure of the element in the mesh, performs refinement of the mesh until requirements on the size of elements are met. A detailed description of the algorithm used by Space is presented in [Meijs 92]. Since the problem of 2D mesh generation is solved, our main concern is the 3D mesh generation. In the subsequent sections we discuss different algorithms which can be used for 3D mesh generation. We study the advantages and disadvantages of these algorithms for the hybrid modeling.

8.4.2 Representation schemes for solid modeling

Various solid modeling techniques have been developed, but only two of them are most relevant to our purposes. The first is called constructive solid modeling (CSG) and the second boundary representation (B-rep) geometric modeling.

The CSG is using primitive solids which are combined with the Boolean set of operations, e.g. union, intersection etc., and geometric transformations to obtain more complex composite objects.

To the advantages of the CSG we may account:

- it allows easy specification of a solid model;
- even with a small number of primitives, quite complicated models can be built;
- it has a simple data structure.

But the CSG is not free of disadvantages. The main disadvantage is the lack of an explicit mathematical definition of the boundary of the domain to be meshed. Thus the CSG is less suited to mesh generation for the boundary element modeling.

The B-rep approach seems to be more suitable for our purposes. The B-rep is based on the observation that a solid object can be completely defined by its boundary elements such as faces, edges and vertices. A vertex is defined as a point in 3D space, an edge is a part of the line, and a face is a bounded part of a surface. Here we have to mention that there are two types of faces:

- simply connected i.e. the boundary of a face consists of a single, closed loop of edges and vertices;
- multiply connected i.e. the boundary of a face may consist of two or more loops, as it is in the case of surfaces containing holes.

In our considerations we use only simply connected faces.

In the B-rep approach, a graph data structure is used to describe the objects by their boundary. The boundary elements are represented by graph nodes and the
The boundary representation of the tetrahedron.

The link between the graph nodes represents the adjacency relationships between the boundary elements.

The graph data structure shows the topology of the objects. It doesn’t change when the geometric transformations are applied to the model. The geometry refers to the location of the boundary elements in the space (the geometric transformation does change it) and it is normally added to the graph data structure by the coordinates of the vertices and/or a parametric description of the faces.

8.5 Mesh generation algorithms

We consider only methods that derive the final mesh, on an element by element bases, from the boundary data. Of these we look at two basic approaches such as advancing-front methods (frontal methods) and algorithms based on the Voronoi-Delaunay construction. These methods create internal points and elements, starting from the boundary of the domain. This boundary is given either in a global manner (for example an analytical definition: equations, splines, Bezier patches, etc.) or in a discrete manner (as a list of the edges or triangular faces approximating the boundary).
8.5.1 The Delaunay method

The Delaunay triangulation/tetrahedrization is a method suited for the local refinement of an existing mesh. In 2D the Delaunay method results in a triangulation of the convex hull of a point set that is in a sense optimal, i.e. it maximizes the sum of the smallest angles over all triangles in the triangulation. Elements with sharp angles are thus avoided as much as possible. The Delaunay triangulation is most easily understood in terms of its dual, the so-called Voronoi tessellation. The Voronoi tessellation of the plane consists of Voronoi polygons $V_i$'s as illustrated in Figure 8.8. Each of polygons $V_i$ corresponds to one of the generating points $P_i$. A Voronoi polygon $V_i$ corresponding to a point $P_i$, contains points of the plane that are closer to $P_i$ than to any other generating point $P_j \neq P_i$. The vertices of the tessellation are the midpoints of the circumscribed circles on the triangles. Each vertex of the tessellation is usually shared by three polygons. Connecting the generating points of the three Voronoi polygons which share the same vertex gives the corresponding Delaunay triangle.

![Figure 8.8. Voronoi tessellation (dot lines) with the corresponding Delaunay triangulation (solid lines), determined by a set of generating points.](image)

It can be easily verified that three points form a Delaunay triangle if, and only if, the circumscribed circle on this triangle doesn’t contain any other generating points. This property is used to create a new Delaunay triangulation when a new point is added to an existing Delaunay triangulation of generating points.

There are many methods to obtain the Delaunay triangulation, e.g.: edge swapping, edge insertion or node insertion. We present the last method, often called Watson’s method.

When a new generating point is added to an existing Delaunay triangulation, the triangles having the new point within their circumscribed circle are determined. The union of these triangles forms the insertion polygon, containing the new point, as it is depicted in Figure 8.9(a). The new triangulation is then formed by connecting
8.5 Mesh generation algorithms

The vertices of the insertion polygon with the new added point, as we illustrate in Figure 8.9(b). Watson’s algorithm can also be used as an algorithm for creating a tetrahedralization in 3D. A Voronoi region $V_i$ is now a solid polyhedron, and each vertex of the polyhedron is usually shared by four polyhedra. The four generating points form a tetrahedron, and the circumscribing sphere of these four points does not contain any of the other generating points. When we want to add a new point, the circumscribed sphere on tetrahedron, belonging to the 3D Delaunay mesh, is used to determine whether this tetrahedron should be included in the insertion polyhedron.

The use of the Delaunay tetrahedralization in 3D, will not necessarily give well-shaped tetrahedra, tetrahedrons with an arbitrarily small volume may be obtained. The Delaunay triangulation/tetrahedralization has the following advantages for FE mesh generation:

- In 2D the triangulation obtained is optimal in the sense that it maximizes the smallest angles.

- The method is suited to the generation of graded meshes and local remeshing.

To the disadvantages of the method we can account:

- In 3D space, badly-shaped tetrahedrons can be generated. They have to be detected and eliminated, but these task are not easy. We can say also that the Delaunay tetrahedralization doesn’t satisfy any optimality criterion.

- The Delaunay triangulation/tetrahedralization is strictly point-based. The convex hull of a point set is triangulated instead of the domain itself. Thus the mesh generated such a way may contain, in the case of the non-convex domain, elements that intersect the boundary.
• A good node generation/insertion strategy is required for the Delaunay tetrahedrization to be applicable for 3D mesh generation.

8.5.2 The Frontal method

This class of methods can be applied to any arbitrary geometry. These methods construct the mesh from its boundary. The elements created are triangles in 2D and tetrahedra in 3D. The data required is the boundary, or more precisely, a polygonal discretization of it in 2D (a list of segments) or a polyhedral discretization in 3D (a list of triangular faces).

The process of mesh generation is iterative: a front, initialized by set of items of the given boundary, is analyzed in order to determine a departure zone, from which one or several internal elements are created. The front is then updated and the element creation is continued as long as the front is not empty.

This process can be summarized as follows:

1. Initialization of the front.
2. Analysis of the front.
   2a. Determination of the departure zone.
   2b. Analysis of this region:
       * Creation of the internal points and internal elements.
       * Update of the front.
3. As long as the front is not empty, go to step 2.

The advancing front method in 2D

The type of mesh generators based on the advancing front method are suitable for any arbitrary geometry. The generated mesh covers up the domain \( \Omega \) by triangles starting from the contour of the domain to be decomposed. In practice a polygonal approximation of the contour is used in terms of a list of its constitutive segments. The interior of the domain and the zone to be meshed, are well defined because of the orientation of the contour provided as data.

The initial front is defined as a set of segments of a boundary \( C \) surrounding the domain \( \Omega \).

Given a front \( F \) associated with the boundary \( C \), we now discuss the manner in which the triangles are created. While the process of the creation of internal triangles progresses, the boundary \( C \) and front \( F \) are updated. Let \( F \) be the current state of the front, then the front analysis is based on the examination of the geometrical properties of the segments that belong to the front \( F \). In Figure 8.10 we show basic cases for the front structure in two dimensions. Let \( \alpha \) be the angle formed by two consecutive segments of front \( F \). The three situations, depending on the value of the angle \( \alpha \), can be defined:
8.5 Mesh generation algorithms

- $\alpha < \frac{\pi}{2}$: the two segments $s_2s_3$ and $s_3s_4$ become the two edges of the single triangle with vertices $\{s_2s_3s_4\}$ created;

- $\frac{\pi}{2} < \alpha < \frac{2\pi}{3}$: from the two segments $s_2s_3$, $s_3s_4$ and a new internal point $s$, the two triangles $\{s_2s_3s\}$ and $\{s_3s_4s\}$ are generated;

- $\frac{2\pi}{3} < \alpha$: one segment $s_2s_3$ of the front is retained and a triangle is created with this segment by adding an internal point $s$.

The position of the internal points created is determined by "optimal" criterion, in the sense that the elements containing these points are as regular as possible. At each point creation, it is necessary to verify that the point is inside the domain in its current state. This means that any point created must be placed inside the domain under consideration and not inside an existing element. This verification is crucial for the frontal method, since it relies on exact knowledge of an adequate neighborhood of the zone under consideration.

A new front is created by removing:

- the edges of the contour, belonging to a triangle created, from the present front;

and by adding:

- the edges of the triangle created which don’t belong to the present boundary.

The advancing front method in 3D

The application of advancing front techniques in the 3D case is obviously more delicate. This technique is still suitable for arbitrary geometries. A mesh generator, again, constructs the covering-up of the domain $\Omega$, this time, by tetrahedra from its boundary data. In practice, a polyhedral approximation of the boundary is used. The boundary description consists then of a list of its constitutive triangular faces. The interior of the domain, namely the region to be meshed, is determined through the orientation of the data.
Implementation of the HEM in the extraction system

The algorithm is based on the same type of scheme as in the 2D case. The process is iterative: from a given contour \( C \) and associated with it front \( F \), the properties of the faces belonging to \( F \) (in terms of size and angle), and their neighborhood are analyzed in order to select a departure zone.

According to the case being considered, either an element is created with the selected faces, or an internal point is generated which allows the creation of the elements by simply joining the internal point to the selected faces. In the 3D case, the condition regarding intersection of the edges is replaced by the two following conditions: the edges resulting from the new internal point should not intersect a face of any element belonging to the front and the faces containing this point are not intersected by any edge of the front.

8.6 Conclusions

A disadvantage of the advancing front method is that it requires geometrical checks to determine whether a newly formed element intersects the generating front. Furthermore, if interior nodes are generated before the element is formed, one must check whether a new element will contain any of these nodes. The conclusion is that the advancing front method is indeed suited to the generation of (also graded) meshes in 2D and 3D, although the method has some disadvantages. One important disadvantage is that the generation of internal nodes and the selection of an internal node have no firm theoretical basis, and there are no optimality criteria to be satisfied. This situation may lead to the creation of badly-shaped elements when the domain to be meshed consists just of few edges or triangles and "collapses" onto itself. In that case, the distances between the nodes have become so small that only nodes on the front itself can be used to create a new element. The selected node may then result in a badly-shaped element.

From the overview of the mesh generation algorithm we conclude that only few of them are suitable for extraction purposes. The algorithm we are looking for should be capable of using the facilities provided by Space, such as already implemented 2D mesh generation and the scanline technique.

It seems that the most suitable for hybrid modeling purposes is the advancing front method for 3D mesh generation. Space with its ability of creating a uniform 2D triangulation mesh on the surface of conductors as well as on the surface of the "inside" region provides the description of the front in the form of the list of triangular elements. The triangles created determine explicitly the interior of the "inside" region by certain orientation of the data. This is achieved by forcing a certain sequence of nodes of the triangular face which determines the normal vector to the face pointing inside or outside of the interior of the domain to be decomposed.

From this contour description the generating points are successively created inside the domain and the creation of tetrahedral elements follows. The departure zone is
8.6 Conclusions

determined by a position of scanline. The 3D elements cover-up the domain till the next scanline position. After creating new tetrahedral element the front is updated. Along with creating a new finite element the calculation of the capacitive model of the element is performed. The contributions of the capacitive elemental models are added to the intermediate capacitance matrix. Once generating node does not belong to the front anymore the relevant row and column in the intermediate capacitance matrix can be reduced.

For the purpose of the implementation of the hybrid method in the package Space we have developed a prototype of the automatic mesh generator based on the advancing front method. This prototype mesh generator has been implemented in the Mathematica package, which offers good visualization facilities. Below we present some of the meshes obtained by using of our prototype mesh generator.

In the second example, illustrated in Figure 8.11, we consider a bit more complex structure. The domain we want to mesh is concave and has non-orthogonal sides. We sweep the structure from left to right with the scan-plane generating the tetrahedrons successively.

The implemented mesh generator has been also tested on more complex boundary meshes obtained from the real layouts. In all cases our generator succeeded in generating of the uniform, well shaped mesh.
Figure 8.11. Successive generation of tetrahedrons in a concave structure with non-orthogonal sides.
Bibliography


A.1 The 2D FEM

Let us consider a domain \( \Omega \) in 2D space in which the Laplace equation is satisfied and the homogeneous Dirichlet boundary conditions are imposed. The domain \( \Omega \) is discretized into, say \( N \), triangular elements.

For a single triangular element, as depicted in Figure A.1, we have

\[
\phi_{V_1} = \frac{A_2 A_3}{A_1} (x - x_1) + \frac{A_1 A_3}{A_2} (y - y_1) + \phi_1
\]

\[
\phi_{V_2} = \frac{A_1 A_3}{A_2} (x - x_2) + \frac{A_2 A_1}{A_3} (y - y_2) + \phi_2
\]

\[
\phi_{V_3} = \frac{A_1 A_2}{A_3} (x - x_3) + \frac{A_3 A_1}{A_2} (y - y_3) + \phi_3
\]

where

- \( A_i \) are the areas of the triangles
- \( x_i, y_i \) are the coordinates of the \( i \)-th vertex
- \( \phi_i \) are the potentials at the vertices
- \( A \) is the area of the element
- \( \sigma \) is the electric conductivity assigned to the element, constant within each element.

Figure A.1. Single triangular finite element in 2D.
Appendix A

THE 2D HYBRID ELEMENT METHOD

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A.1 The 2D FEM

Let us consider a domain $\Omega$ in 2D space in which the Laplace equation is satisfied and the inhomogeneous Dirichlet boundary conditions are imposed. The domain $\Omega$ is discretized into, say $N$, triangular elements.

For a single triangular element, as depicted in Figure A.1, we have:

$$(x_{i}, y_{i})_{i=1,2,3}$$ - the coordinates of the three vertices of the triangle;
$$\phi_{1}, \phi_{2}, \phi_{3}$$ - the potentials at the vertices of the element;
$$\Delta$$ - the area of the element;
$$k$$ - the dielectric permittivity assigned to the element, constant within each element.

Figure A.1. Single triangular finite element in 2D.
We assume that the potential within the element is approximated by an (affine) linear expression:

$$\phi^e(x, y) = \alpha_1 + \alpha_2 x + \alpha_3 y = \begin{bmatrix} 1 & x & y \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix}^T \quad (A.1)$$

To obtain the constant coefficients $\alpha_1$, $\alpha_2$ and $\alpha_3$, we solve the following set of equations:

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} \quad (A.2)$$

which matches the potentials in the nodes of the element.

Substituting (A.2) into (A.1) we obtain:

$$\phi^e(x, y) = \begin{bmatrix} 1 & x & y \end{bmatrix} \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}^{-1} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} f_1(x, y) \\ f_2(x, y) \\ f_3(x, y) \end{bmatrix}^T \quad (A.3)$$

Here, functions $f_1(x, y)$, $f_2(x, y)$, $f_3(x, y)$ are the local shape functions such that:

$$\begin{bmatrix} f_1(x, y) \\ f_2(x, y) \\ f_3(x, y) \end{bmatrix} = \begin{bmatrix} 1 & x & y \end{bmatrix} \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ y \end{bmatrix} \quad (A.4)$$

with

$$\Delta^e = \frac{1}{2}[(x_2 y_3 - x_3 y_2) + (x_3 y_1 - x_1 y_3) + (x_1 y_2 - x_2 y_1)] \quad (A.5)$$

Using the energy approach described in Chapter 3 we derive the following set of equations:

$$\begin{bmatrix} C_{11}^e & C_{12}^e & C_{13}^e \\ C_{21}^e & C_{22}^e & C_{23}^e \\ C_{31}^e & C_{32}^e & C_{33}^e \end{bmatrix} \begin{bmatrix} \phi_1^e \\ \phi_2^e \\ \phi_3^e \end{bmatrix} = \begin{bmatrix} \delta_1^e \\ \delta_2^e \\ \delta_3^e \end{bmatrix} \quad (A.6)$$

with

$$C_{ij}^e = \int_{\Delta^e} k e \left[ \frac{\partial f_i}{\partial x} \frac{\partial f_j}{\partial x} + \frac{\partial f_i}{\partial y} \frac{\partial f_j}{\partial y} \right] dx \, dy \quad (A.7)$$

The equivalent capacitance network for a single element is shown in Figure A.2.

The relationship between elements of the network and the entries of the capacitance matrix $C^e$ is as follows:

$$\begin{bmatrix} (C_{12} + C_{13}) & -C_{12} & -C_{13} \\ -C_{12} & (C_{12} + C_{23}) & -C_{23} \\ -C_{13} & -C_{23} & (C_{13} + C_{23}) \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \end{bmatrix} \quad (A.8)$$
Figure A.2. The equivalent capacitance network for a single triangular element.

where

\[ C_{12} = \frac{1}{4\Delta_e} [(y_3 - y_2)(y_3 - y_1) + (x_2 - x_3)(x_1 - x_3)] \]  \hspace{1cm} (A.9)

\[ C_{13} = \frac{1}{4\Delta_e} [(y_2 - y_3)(y_2 - y_1) + (x_3 - x_2)(x_1 - x_2)] \]  \hspace{1cm} (A.10)

\[ C_{23} = \frac{1}{4\Delta_e} [(y_1 - y_3)(y_1 - y_2) + (x_3 - x_1)(x_2 - x_1)] \]  \hspace{1cm} (A.11)

A.2 The transformers at the boundary interface in 2D

In the 2D case the boundary interface between the “outside” and “inside” region consists of edges.

For each edge on the interface boundary we have:

Outside: an average edge potential \( \Phi_i \) and a constant charge \( \sigma_i \) for an edge \( i \);

Inside: a node potential \( \phi_\alpha \) and an overall node charge \( \delta_\alpha \) for a node \( \alpha \).

For each edge on the boundary interface we determine the center of gravity which is simply the center of an edge and divide it in two half-edges. We distribute the “outside” charge on edge \( i \) evenly over the two end nodes of the edge, yielding for the case shown in Figure A.3:

\[ \delta_\alpha = \frac{1}{2} [\sigma_j + \sigma_k] \]  \hspace{1cm} (A.12)

For the potential, referring to Figure A.3, we assume that each \( \Phi_j \) is the average of the node potentials belonging to its edge \( j \):

\[ \Phi_j = \frac{1}{2} [\phi_\alpha + \phi_\beta] \]  \hspace{1cm} (A.13)

This leads, in general, to the transformer equation:
The 2D hybrid element method

We assume that the potential within the element is described by an affine linear expression

\begin{equation}
\phi(x) = \sum_{i=1}^{n} a_i \phi_i(x)
\end{equation}

To obtain the constant coefficients, we solve the following set of equations.

\begin{align}
\delta_b &= T \sigma_b \\
F_b &= T^T \phi_b
\end{align}

Here, the index 'b' denotes the boundary interface and \( T \) is the transformer matrix. The matrix \( T \) is sparse and such that \( T_{ij} = \frac{1}{2} \) if the \( i \)th boundary node belongs to the \( j \)th boundary edge, and 0 otherwise.
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Parasitic interconnect capacitances in integrated circuits (IC's) are playing an increasingly significant role in the circuit's performance. Therefore, designers of modern IC's rely heavily on layout-to-circuit extraction systems, which produce an equivalent electrical model from the layout. Subsequent simulation verifies correct behavior of the circuit before costly fabrication.

Until now, the boundary element method (BEM) and the finite element method (FEM) are the most popular techniques used for capacitance modeling. The BEM is based on the assumption that the structure of IC's may be well approximated by a uniform stratification of dielectric layers, as is shown in Figure S.1, bordered at the bottom by ideal ground plane, whose potential is zero. The conductors running through such a dielectric structure are assumed to be perfectly conducting and each of them forms an equipotential.

The BEM, for calculation of multiconductor capacitances, allows to express the electrostatic potential in terms of the prime integrals known in the form of Green's function. However, the BEM can only be used when the Green's function is readily given, i.e. when the stratification of the dielectric layers is perfect. If the dielectric structure of the integrated circuit becomes irregular, as in Figure S.2, the Green's
function method loses much of its usefulness. Then one must resort to the FEM which solves the differential equations in a closed, relatively small domain directly and locally. But the FEM results in a very large system of linear equations when it models the entire layout of IC. The other disadvantage of the FEM, in comparison with the BEM, is that it cannot handle the effects of an electrical field which extends to infinity.

Figure S.2. Example of the disturbed stratification.

In this thesis we propose the hybrid element method (HEM) for the modeling of capacitive interconnects, which is capable of dealing with disturbances and/or irregularities in a dielectric stratification. The main idea behind our method is to combine the BEM and the FEM in one capacitance extraction system, so that the BEM is used in the regular regions of the layout of IC, while the FEM is used in the bounded, localized regions that exhibits irregularities. The derivation of the capacitance models for either the BEM or the FEM is well known, we recall them shortly in Chapter 2 and Chapter 3, respectively.

The main modeling problem we consider in this thesis is how to connect the two models obtained by the BEM and the FEM.

Some proposals for the hybrid BEM/FEM method can be found in the literature. However, they focus on solving particular field problems and do not give a good physical circuit model, which is desired for extraction purposes.

Our proposal for the electrical model of the interface between regions modeled by the BEM and the FEM is a generalized ideal transformer, we explain its derivation in Chapter 4, and obtain a complete circuit model consisting of a lossless system of capacitances coupled by ideal transformers. Elimination of the transformers yields a purely capacitive model. From this model we can easily derive all the capacitive couplings and we can select a number of the most strongly coupled pairs of conductors for further analysis and/or redesign process.

We discuss the convergence of the hybrid method in Chapter 5. We show that the energy associated with the discontinuity of the field at the boundary interface contributes a negligible part to the total energy, namely a part that goes to zero quadratically as the mesh gets finer.
The hybrid method has been validated and tested for basic benchmarks with layered media in two and three dimensions. Theoretically we found good convergence properties of the hybrid method. These have been confirmed by the practical results, which we present in Chapter 6. Comparison of results obtained by the HEM and by other methods shows the usefulness and superiority of the hybrid method.

In Chapter 7, we consider possible extensions and applications of the HEM to other problems than capacitance extraction.

In Chapter 8, we present a prototype implementation of the HEM capable of handling simple geometries. Finally, we discuss how the method can be integrated in a modern extraction system like Space.
De aanwezigheid van parasitaire capaciteiten in geïntegreerde schakelingen (IC's) speelt een steeds belangrijker wordende rol in de prestatie van die schakelingen. Ontwerpers van hedendaagse IC's steunen in belangrijke mate op zogeheten "layout-to-circuit" extractie systemen, die een equivalent elektrisch model opleveren van de layout van het IC inclusief de parasitaire capaciteiten. Door middel van simulaties aan dit model kan de correcte werking van het IC worden geverifieerd, alvorens de zeer kostbare fabricage wordt ondernomen.

\[ C_{12} = C_{21} \]

**Figure S.3.** De doorsnede van de layout met twee geleiders en hun capacitieve koppelingen.

Tot op heden geldt dat de grensvlak elementen methode (boundary element method, afgekort BEM) en de eindige elementen methode (finite element method, afgekort FEM) de technieken zijn bij uitstek voor het modelleren van capaciteiten. De BEM is gebaseerd op de aanname dat de diëlektrische structuur van een geïntegreerd circuit kan worden benaderd door een uniforme stratificatie van de diëlektrische laggen, zoals geïllustreerd in Figuur S.3, aan de onderzijde begrensd door een ideaal geleidend aardingsvlak, waarvan het potentiaal gelijk is aan nul. Verder wordt er van uitgegaan dat de geleiders die zich in zo'n diëlektrische structuur bevinden, allen perfect geleidend zijn en elk een equipotentiaal vormen.

De BEM staat het toe om, voor de berekening van de multi-conductor capaciteiten,
Samenvatting
de elektrostatische potentiaal uit te drukken in termen van integraalvergelijkingen gebaseerd op de zogeheten Green'se functie. De BEM kan echter alleen worden gebruikt als de Green'se functie berekend kan worden, wat slechts realistisch is als de stratificatie van de diëlektrische lagen perfect is. Zodra de structuur van het IC onregelmatig is, zoals geïllustreerd in Figuur S.4, verliest deze methode veel van zijn nut. Men moet zich dan richten op de FEM, die de differentiaalvergelijkingen op een lokale en directe wijze oplost voor een relatief klein en begrensdbied. Echter, het toepassen van de FEM op de gehele layout van het IC resulteert in een extreem groot systeem van lineaire vergelijkingen. Tevens is het zo dat de FEM, in vergelijking tot de BEM, de effecten van het elektrische veld in het oneindige niet goed aankan.

\[ k_3 \]
\[ k_2 \]
\[ k_1 \]

**ground plane**

**Figure S.4.** Voorbeeld van een verstoorde stratificatie.

In dit proefschrift stellen wij een hybride elementen methode (hybrid element method, afgekort HEM) voor die geschikt is om overweg te kunnen met verstoringen van- of onregelmatigheden in de diëlektrische stratificatie. De hoofdgedachte achter onze methode is een combinatie van beide methodes te vormen, waarin de BEM wordt toegepast in de regelmatige gebieden van de layout, en de FEM slechts wordt toegepast in de lokale, begrensde gebieden waarin de onregelmatigheden zich bevinden. Het gebruik van de BEM of FEM om vanuit de layout tot het capaciteitsmodel te komen is welbekend, en wordt in de Hoofdstukken 2 en 3 aan de orde gebracht.

Het modelleringsprobleem dat wij in dit proefschrift als hoofdzaak behandelen is de koppeling tussen de capaciteitsmodellen die door de beide methodes (BEM en FEM) worden geleverd.

In de literatuur kan men een aantal andere voorstellen vinden voor hybride methodes gebaseerd op de FEM en BEM. Echter, deze richten zich op het oplossen van bepaalde veldproblemen en leveren geen werkbare fysisch model van de schakeling op, wat onze doelstelling is.

Ons voorstel voor het model van de koppeling in het scheidingsvlak tussen de gebieden die door beide methodes worden gemodelleerd, is dat van een gegeneraliseerde ideale transformator. In Hoofdstuk 4 geven wij een afleiding hiervoor, met als resultaat dat het model voor de gehele schakeling dat is van een verliesvrij systeem van capaciteiten en ideale transformatoren. Deze transformatoren laten zich
vervolgens elimineren, wat leidt tot een puur capacitief model. De belangrijkste van deze capaciteiten kunnen in beschouwing worden genomen voor verdere analyse en/of herontwerp van het IC.

In Hoofdstuk 5 beschouwen we de convergentie van de voorgestelde hybride methode. Hierin tonen wij aan dat de energie die gerelateerd is aan de discontinuïteit van het veld in het scheidingsvlak verwaarloosbaar klein is ten opzichte van de totale energie, en dat deze tevens kwadratisch kleiner wordt met het verfijnen van de discretisatie.

De hybride methode is gevalideerd en getest voor een aantal eenvoudige benchmarks met gelaagde media, in zowel twee als in drie dimensies. In Hoofdstuk 6 presenteren wij de resultaten van praktische experimenten die de theoretisch goede convergentie eigenschappen bevestigen. Vergelijking van de resultaten van de HEM met die van de andere methoden toont aan dat de hybride methode superieur is.

In Hoofdstuk 7 overwegen wij mogelijke uitbreidingen en toepassingen van de HEM op andere problemen dan het modelleren van capaciteiten.

In Hoofdstuk 8 tonen wij een prototype implementatie van de HEM die eenvoudige geometriën aankan. Als laatste bespreken wij hoe deze methode optimaal kan worden opgenomen binnen een modern layout-to-circuit extractie pakket zoals Space.
Samenvatting
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[Text is not visible, likely due to image quality or page format issues.]
Ewa Barbara Nowacka was born on December 27th, 1968 in Choszczno, Poland. In June 1987, she received her Lyceum diploma with honours at “Władysław IV” Lyceum in Warsaw, Poland. In October the same year she started her studies in electrical engineering at the Warsaw University of Technology, Dept. of Electrical Engineering, Institute of Electronic Fundamentals. In 1990 she started her specialization at the Network Theory Section, working on simulation techniques for integrated circuits. The last year of her studies she has spent at the Delft University of Technology, Network Theory Section where, under supervision of Prof. P.M. Dewilde, she has carried out her Master’s research. Her Master’s thesis dealt with modeling of parasitic capacitances in integrated circuits. In September 1992, she received her M.Sc. degree (cum laude) from the Warsaw University of Technology. In October 1992, she joined the Network Theory Section at the Delft University of Technology as a Ph.D. student. During her four year stay there, she has been involved in the Space project, continuing her research started during her Master’s studies. The main domain of her interest was developing new techniques for modeling of parasitic capacitances in VLSI circuits.

In October 1996, she joined the Digital Signal Processing Group of the Philips Research Labs (NatLab) in Eindhoven. Her new field of interest is in channel coding with particular emphasis on turbo coding.
1. The key concept of our hybrid element method (HEM) is to combine the boundary element method (BEM) and the finite element method (FEM) in one capacitance extraction system, so that the BEM is used in the regular regions of the layout of the IC, while the FEM is used in bounded, localized regions that exhibit irregularities. The HEM profits from the advantages of both the BEM and the FEM and avoids their disadvantages.

2. Our proposal for the electrical model of the interface between regions modeled by the BEM and the FEM is a generalized ideal transformer. The transformer provides for an ideal lossless coupling between the capacitive models resulting from the BEM and the FEM.

3. In contrast to the known direct methods, we satisfy the continuity conditions between the regions modeled by the BEM and the FEM in an average sense by imposing certain potential and charge distributions. This produces an essential singularity in the gradient of the field which, however, contributes only a negligible part to the total energy, namely a part that goes to zero as $O(h^2)$ ($h$ the size of the mesh) when the mesh refines.

4. Important for the successful integration of the HEM, presented in this thesis, in the extraction package Space, is the co-development of a good 3D-mesh generation scheme matching the HEM as well as the scanline technique of Space.
5. Even if it might often look that everything has been discovered, valuable new results can be achieved by the synthesis of several old ones. This is particularly true for the HEM presented in this thesis.

6. Successful research is due at least as much to the choice of the topic as to the quality of the research itself.

   after P.M. Dewilde

7. The successful interfacing of Space to design packages of other EDA vendors will greatly increase its commercial success.

8. Those who plan their conferences in exotic locations should put extra effort to keep their conference more attractive than the place where it is held.

9. The presence of the Internet and the World-Wide Web (WWW) is a mixed blessing. While it makes it easier to find people "on the web" who are sharing the same (professional) interest, others can (mis)use it to find you. This is where the Internet terror may start.

10. People are willing to buy a household product rather for the fact that its exterior has been designed by a famous designer than for its functionality or ease of use.

11. It is a paradox that the brain is functioning as a formidable computer, since it has such a weak memory. The information received is not stored as is, the system filters, selects and changes it. This behavior is due to processing, and the result of what comes out of the memory is in all probability not the same as what went in.

   The Mechanism of Mind
   by Edward de Bono
   translated back to English from Dutch

12. When there is a hill to climb, don't think that waiting will make it smaller.

   Life's Little Instruction Book
   by H. Jackson Brown, Jr.

13. Never give up on what you really want to do.

   Life's Little Instruction Book
   by H. Jackson Brown, Jr.

14. Nothing in Polish sounds the same as in Dutch.

   "nic" phonetically equals "niets"