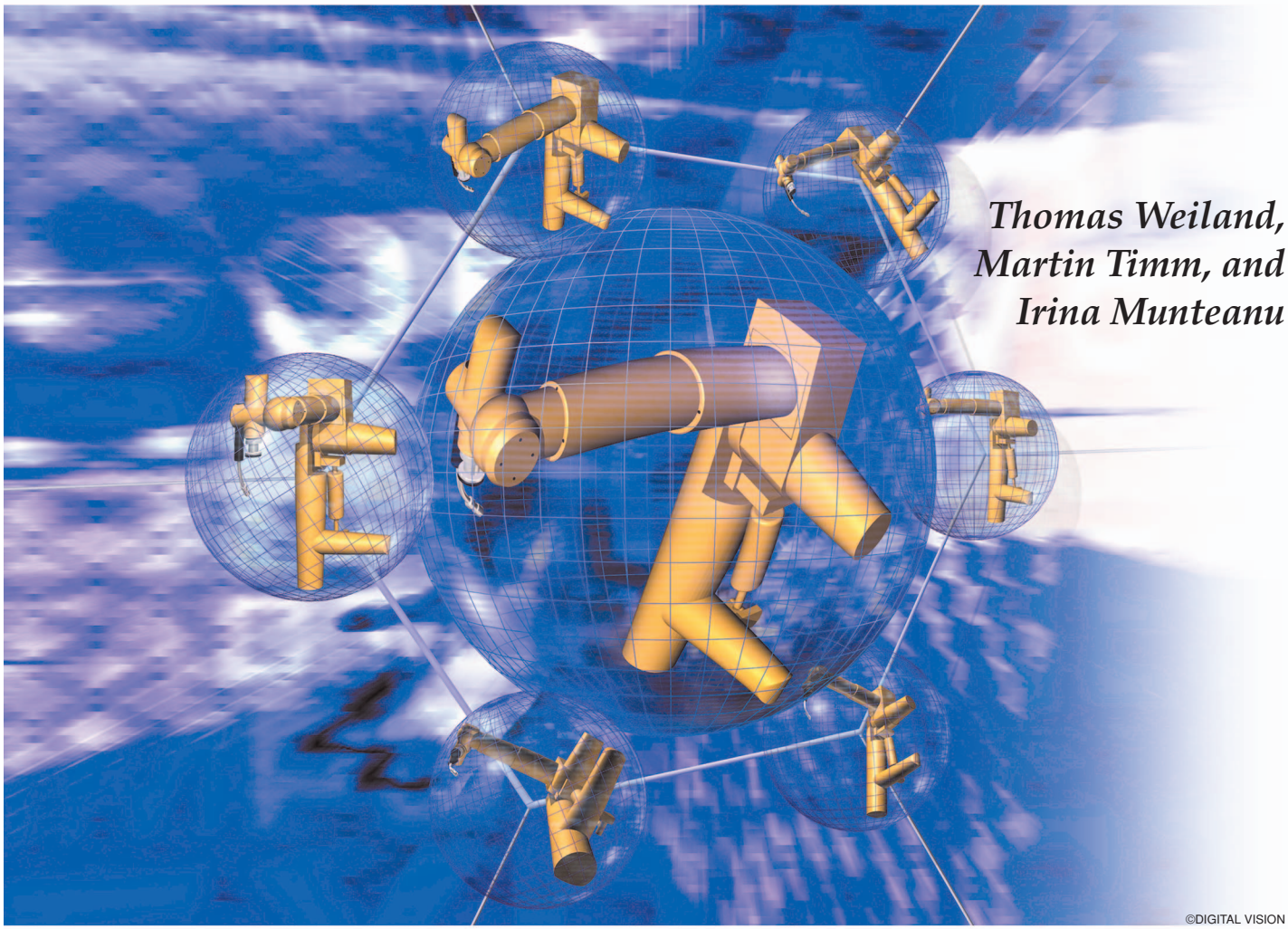
A Practical Guide to 3-D Simulation



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This article is intended to give design engineers an overview over some properties of numerical methods used in today's most relevant commercial electromagnetic (EM) simulation tools. It cannot and does not want to be a rigorous analysis of the methods themselves nor a concise description of their history. For an extensive overview, we would recommend textbooks such as [1] and [2]. The authors have experience in not only the research and development (R&D) of numerical methods but also in the support of users in their daily work with commercial simulation software.

Designing passive components, whether it is obvious or not, is all about solving Maxwell's equations. From university, we know that the pen and paper approach for finding appropriate solutions is very limited: in complex systems, complicated differential equations can not be solved

by analytical methods. Designers typically circumvent this problem by simplification. Often empirical models are used that replace reality, for example, by introducing circuit elements. These models typically have a limited range of validity, which is easily disregarded while using them. In this article, we will deal with three-dimensional (3-D) volume based numerical methods. Their advantage is that they have very little physical constraints in their application range. Even though a single numerical field simulation requires much more time and computing resources than a circuit simulation, this additional deployment of resources might be well invested.

It is widely accepted that 3-D numerical simulations of EM fields are essential to the success of an R&D department working predominantly on passive components. Obviously, simulating a virtual prototype is much cheaper than building hardware and measuring it, in particular if the design cycle time is considered as well. Looking at modern optimized antenna designs, for example, it is arguable whether this design would have been possible at all without EM field simulation tools, without automatic optimization, without the possibility to visualize the previously invisible. But saying, "all right, let's go and buy a 3-D EM field simulator and everything will be fine" is probably not sufficient. We want to discuss the pros and cons of different methods here, as well as give some hints on how to use such simulators.

Solving Maxwell's Equations

All numerical approaches to solve Maxwell's equations partition space into subdomains, where solutions can be found more easily. A mode-matching code, in its simplest application, composes a waveguide system from sections with known behavior by performing a modal expansion and matching the fields at the intersection areas. A method-of-moments (MoM) code synthesizes the far field of an antenna by integrating the Green's functions of single metallic surface patches. Volume discretization methods work with even more brute force. They subdivide space into small cells and apply Maxwell's equations on each such entity. To solve the full problem, all single-entity solutions are summed up in a usually large system of equations, which needs to be tackled in one way or another.

When discussing the properties of the different methods, it is necessary to classify them. A major point of difference is the domain they are working in, which is either time domain or frequency domain. Concentrating on the methods that are most relevant commercially, we find on the time domain side the finite integration technique (FIT) (see "Finite Integration Technique" [3], [4]); finite difference time domain (FDTD) in its explicit [5], [6] or implicit [7], [8] variants; and the transmission line matrix (TLM) method [9], [10]. The frequency domain is represented by the finite element method [11], [12]; FIT; and the MoM [13]. All methods are volume discretization methods, except for the MoM, which is a surface discretization method.

A Typical Model Set-Up

In setting up a computer model for a real device, there are several steps, which are common to all discussed simulation methods. All of them bear risks to introduce errors into the simulation, i.e., discrepancies between simulation results and measurements. A typical model setup is demonstrated in the following, using the example of a rather simple 90° coaxial connector (Figure 1).

First of all, a geometrical model needs to be created. This can be either done by using a modeler built into the simulation software or by importing the geometrical data from a mechanical CAD tool. Importing from CAD tools is not as easy as it sounds, and the quality of import filters varies significantly; but this is beyond the scope of this article. If comparing to an existing device, the exact same dimensions have to be used. Sounds simple? Besides obvious errors, there are always tolerances, and sometimes details are neglected, which are relevant at microwave frequencies and radiofrequency (RF).

The considered connector is assembled from different materials, like polytetrafluoroethylene (PTFE, Teflon), copper, etc. Knowledge of the exact material properties is essential for an accurate simulation, but this is normally not available.

The computational effort for volume-based methods depends also on the volume size, and the size of the simulation model must always be finite, even if in reality the component is placed in an infinite surrounding. In order to reduce surrounding space, boundary conditions need to be introduced that represent, for example, electric walls, free space, symmetry, or periodicity. For our connector, this is not relevant, because we can simply assume that the space surrounding it is a perfect conductor, as we know that there will be virtually no field penetrating the conductor shielding.

Finally, we have to define *ports* in the model to excite the structure and to monitor simulation results such as transmission and reflection. Ideally, these ports should not have an impact on the simulation results.

Performing a Simulation

Having set up our geometrical representation of the real structure in the software environment, we can now start the steps towards the final results. The first step is the actual space discretization—the mesh setup—which is automated to a large extent in modern commercial software. Despite the high degree of automation, the proposed mesh might need to be checked or influenced manually in order to obtain accurate results. In a second step, the software creates the system matrices based on the geometrical information from this grid and the method chosen for approximating Maxwell's equations. After all the required matrices are created and assembled, the third step starts; namely the solution of the finite algebraic system. Here we want to calculate the S-parameters for our connector, since they are the most often requested result for passive component characterization.

In the frequency domain, this process is straightforward [Figure 2(b)]: one simulation delivers the S-parameters at one frequency point. However, the behavior is usually relevant in a specified frequency range, so looking at a single frequency is not sufficient. Therefore, a number of simulations in the frequency band of interest have to be performed. Special algorithms are used to minimize the number of simulations required to achieve a predefined accuracy by interpolating the S-parameters in between the simulated frequency points. In the case of our connector, ten simulations are necessary to cover the range of 0–8 GHz with a predefined accuracy of 1% over the entire frequency band.

In time domain, the approach is quite different [Figure 2(a)]. The user specifies the frequency range of interest (e.g., 0–8 GHz). A Gaussian signal $X(f)$ covering this frequency range is defined. This spectrum is then transformed into time domain by using an inverse Fourier transformation, resulting in a time signal $x(t)$

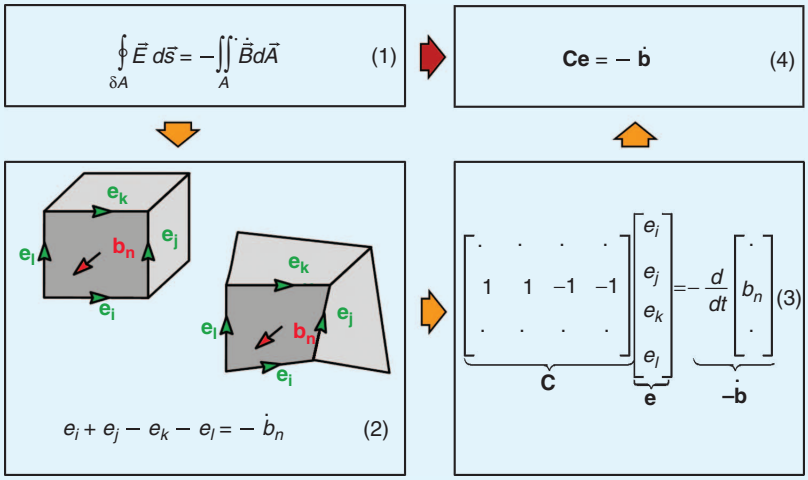
Finite Integration Technique

The Finite Integration Technique gets its name from the fact that it discretizes the *integral* rather than the differential form of Maxwell's equations. The unknowns are the electric voltages, denoted by $\mathbf{e}$, on the edges of the discretization mesh and the magnetic fluxes, denoted by $\mathbf{b}$, on the mesh faces.

For discretizing Faraday's law (1) on a mesh face, for instance, we note that the left hand side of (1) is a line integral of the electric field (i.e., an electric voltage) along the border of the face. This integral can be simply written as an algebraic sum of the edge unknowns. The right hand side is nothing else than the time derivative (denoted by a dot) of the magnetic flux through the face. Note that, for any fixed mesh (which already includes a space discretization error), no supplementary equation discretization error is involved, when passing from the continuous to the discrete form. This is because, with this choice of unknowns, the passage from (1) to (2) is based solely on the mathematical properties of the integral. On the other hand, an equation discretization error will occur when discretizing the material property relations.

By grouping the $+1$ and -1 coefficients of the algebraic sum into a matrix $\mathbf{C}$ (the discrete counterpart of the curl operator), and the electric and magnetic unknowns in vectors $\mathbf{e}$ and $\mathbf{b}$, a compact matrix form results, which looks strikingly similar to the continuous differential form of Faraday's law $curl\vec{E} = -\dot{\vec{B}}$.

In a similar way, all Maxwell's equations can be discretized with the FIT to yield their discrete counterparts, with a compact and elegant matrix form [3]. The matrix operators $\mathbf{C}$, $\tilde{\mathbf{C}}$ (the discrete curl operators) and $\mathbf{S}$, $\tilde{\mathbf{S}}$ (the discrete divergence operators) are topological matrices, containing only $\mathbf{1}$, $-\mathbf{1}$ and 0 entries. On a Cartesian grid, FDTD is equivalent to the FIT [4]. Even the modern view on the FEM method uses exactly the same form (6) of discretized Maxwell's equations [11]. The difference between modern FEM and FIT is only in the discretization of the material property relations.



$$\oint_{\partial A} \vec{E}\cdot d\vec{s} = -\frac{\partial}{\partial t}\iint_{A} \vec{B}\cdot d\vec{A} \qquad \mathbf{Ce} = -\dot{\mathbf{b}}$$

$$\oint_{\partial A} \vec{H}\cdot d\vec{s} = \iint_{A}\left(\frac{\partial \vec{D}}{\partial t} + \vec{J}\right)\cdot d\vec{A} \quad (5) \qquad \tilde{\mathbf{C}}\mathbf{h} = \dot{\mathbf{d}} + \mathbf{j} \quad (6)$$

$$\oiint_{\partial V} \vec{B}\cdot d\vec{A} = 0 \qquad \tilde{\mathbf{S}}\mathbf{d} = \mathbf{q}$$

$$\oiint_{\partial V} \vec{D}\cdot d\vec{A} = Q \qquad \mathbf{Sb} = \mathbf{0}$$

with a Gaussian envelope. The mode pattern at the input port is then excited with this time pattern and propagated through the structure. Reflected and transmitted time signals, denoted generically by $y(t)$, are monitored and after the simulation is ready, a Fourier transform is applied to yield the respective spectra $Y(f)$. These spectra are eventually divided by the excitation spectrum, et voilà: the S-parameters for the entire frequency range in one single go!

The accuracy of a simulation, namely the accordance of simulation results and the behavior in reality, is usually limited due to simplifications in the simulation model. Having the simulation results in front of us, we may wonder whether these are the true S-parameter of our device. All numerical methods promise that the simulation results will eventually converge against the actual solution, if only the mesh is fine enough and all details and effects are represented in the numerical model. If the results of interest do not change significantly anymore after several mesh refinement steps, the converged solution has been reached. Cross verification of the results by applying two different numerical approaches to the same problem gives even more confidence, e.g., by comparing the time domain solution and frequency domain solutions (Figure 3). This reassurance

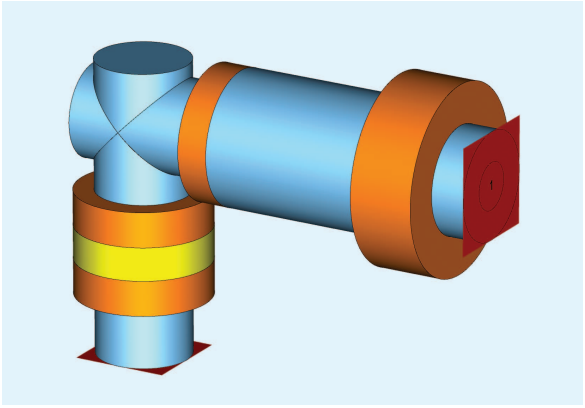


Figure 1. *Simulation model of a 90° coaxial connector. The white space around the connector is perfectly electric conducting. The different colors denote different materials (blue: air, orange: Teflon, yellow: rubber). The ports are already attached (red faces).*

is even more convenient to reach, if the simulation software offers the possibility to switch between numerical approaches without changing the interface.

As we can see in Figure 3, both approaches, frequency and time domain, deliver the same results. There is just another constraint, which has not yet been

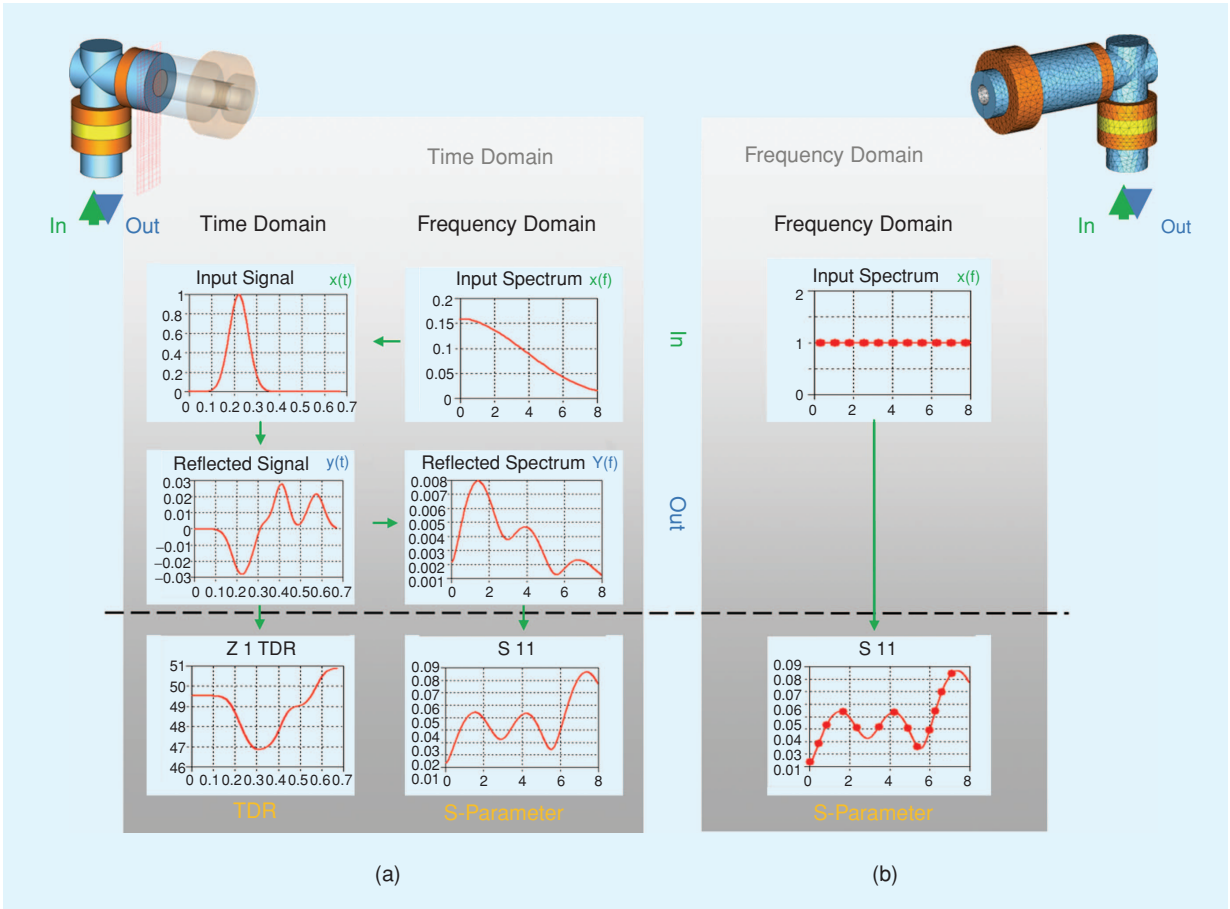


Figure 2. *Schematic of the simulation procedure to derive the S-parameters of a passive component in (a) time and (b) frequency domain. The time signals can also be used to perform a time domain reflectrometry (TDR) analysis of the structure.*

considered—the simulation performance. It is defined by the time required for a simulator to reach a predefined accuracy. For our connector, the simulation time does not differ much between a FIT transient solver (1 min) versus a FIT-FEM frequency domain solver (1.5 min). However, for other applications, the difference in computing time may be significant.

In order to find the most efficient numerical solution for a certain application, it is essential to understand the methods in more detail.

Time Domain

All time domain methods that we are discussing here—FIT, FDTD, and TLM—feature a Cartesian (or cuboid hexahedral or circular cylindrical coordinate) grid and an explicit time integration scheme. These two facts are closely related. The coordinate grid implicates a simple band structure of the system matrix on which the leap frog algorithm can be applied [5]. The fields are propagated through the structure by matrix vector multiplications with a specific time step. The larger the time step, the shorter the simulation time. The maximum possible time step is determined by the Courant-Friedrich-Lewy (CFL)-criterion [14], [27]. It is basically the time required for light to pass the smallest mesh cell in the calculation domain. It might be more illustrative to think of the CFL-criterion as a way to force information from a mesh cell to touch every neighbored mesh cell in every time step. The memory requirements and the simulation time increase linearly with the number of mesh points. Because of these properties, time domain simulators are well suited to solve electrically large and detail-rich structures. Billions of unknowns have been practically demonstrated.

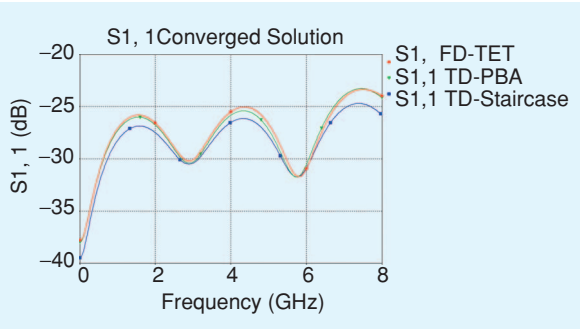


Figure 3. *S-parameters of the connector example derived with different solution methods: 1. Frequency domain solver on a tetrahedral grid with 0.150 million tetrahedra (FD-TET). 2. Time domain solver with PBA on a hexahedral grid with 0.7 million mesh cells (TD-PBA). 3. Time domain solver/staircase on a hexahedral grid with 17 million cells (TD-Staircase). The comparison shows good agreement between cases 1 and 2.*

There are other time domain approaches that use nonorthogonal grids [28] and/or implicit time integration schemes [7], [8]. In the area of microwave and RF, there are currently no commercial implementations available. An implicit algorithm always has to solve a system of equations for every time step, but then the time step size may be chosen somewhat larger.

As we have seen, it is possible to derive frequency domain data by applying Fourier transforms to the time domain signals. Steady-state 3-D EM fields can also very easily be extracted from the transient broadband simulation. Since the excitation signal is broadband, it is possible to obtain fields for various frequencies in one simulation run. Two typical applications shall be mentioned briefly. The first one is a wideband dual ridged horn antenna. Farfields at 100 different frequencies are calculated in one single simulation run to evaluate the broadband gain (Figure 4). The second one is a multiband mobile phone antenna next to a human head model. Here it is also important to model the frequency dependent behavior of the biological tissues correctly.

Time domain naturally offers the possibility to study the transient behavior of EM structures. For this purpose it is not necessary to stick to the Gaussian pulse that has been introduced earlier. Arbitrary signals can be fed into the simulator. (The approach to excite a sinusoidal signal in time domain in order to obtain the harmonic results at the specified frequency is somewhat outdated.) In addition to being used as virtual network analyzer, the simulator can also work as virtual time domain reflectometer (TDR), Figure 2. Delay times and signal degradation on signal lines can be directly simulated.

Not only the signals, but also fields can be studied in time domain: e.g., transient farfields become increasingly important in ultrawide-band (UWB) applications. In multiport devices, every port can be excited individually with a different time signal, and the fields can be monitored accordingly.

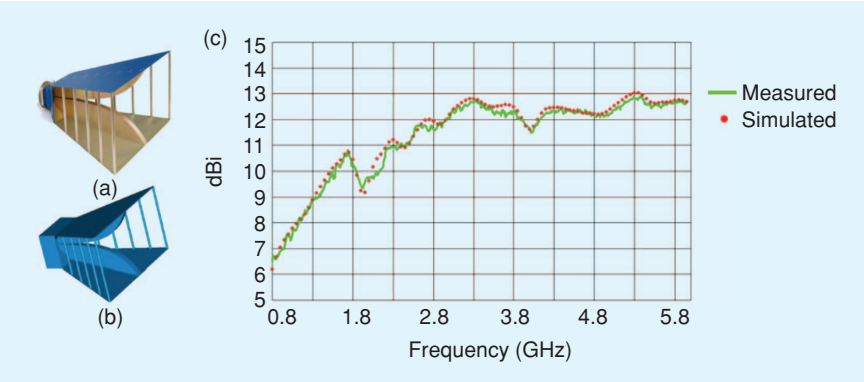


Figure 4. *Broadband simulation of a dual ridged horn antenna [22]. Farfields at 100 frequencies are extracted in one single simulation run by applying broadband time domain technique.*

Geometry Approximation in Time Domain Methods

In traditional FDTD and TLM methods, every hexahedral mesh cell is filled entirely with one material. This leads to the so-called staircase approximation of the geometry. Obviously, such a discretization can make the accurate geometrical representation of many practical devices very difficult, since most components contain rounded features. In order to increase the accuracy in such cases, very fine meshing needs to be applied. Conformal methods, such as the Perfect Boundary Approximation (PBA) [20], can improve the geometry description without compromising the memory efficiency of standard FDTD [6]. The performance increase through such a method is remarkable, as we can also see in our connector example (Figure 5). Not only is a smaller number of mesh cells needed, but the larger mesh cells additionally entail a larger time step. Finally, it is interesting to see how the results converge to a final solution when the mesh is refined. The PBA convergence process is very smooth and extraordinarily fast [Figure 5(a)]; it can be confidently assumed that every increase in mesh density will improve the result's accuracy. This statement is not true for staircase approximations where convergence is slow and not steady [Figure 5(b)].

Endeavors have been made to improve the geometry approximation inside the Cartesian grid. PBA, for example, can also be used to model finite-thickness metallization within one mesh cell. This would result in tiny mesh cells in traditional FDTD and vice versa to very small timesteps and long simulation times. In TLM, however, even more advanced compact models can be found. Fine structured elements like slots, vents, or cables are replaced by specific macromodels in order to avoid the sampling of all details by the grid. This approach has been proven particularly useful in EMC applications (Figure 6).

The standard FDTD grid is structured. This means that every mesh line starts on one side of the calculation domain and ends on the other side. In order to avoid the increase of mesh cells in the outer regions, subgridding algorithms have been introduced, which allow locally smaller mesh cells. The mesh cells need only to be small

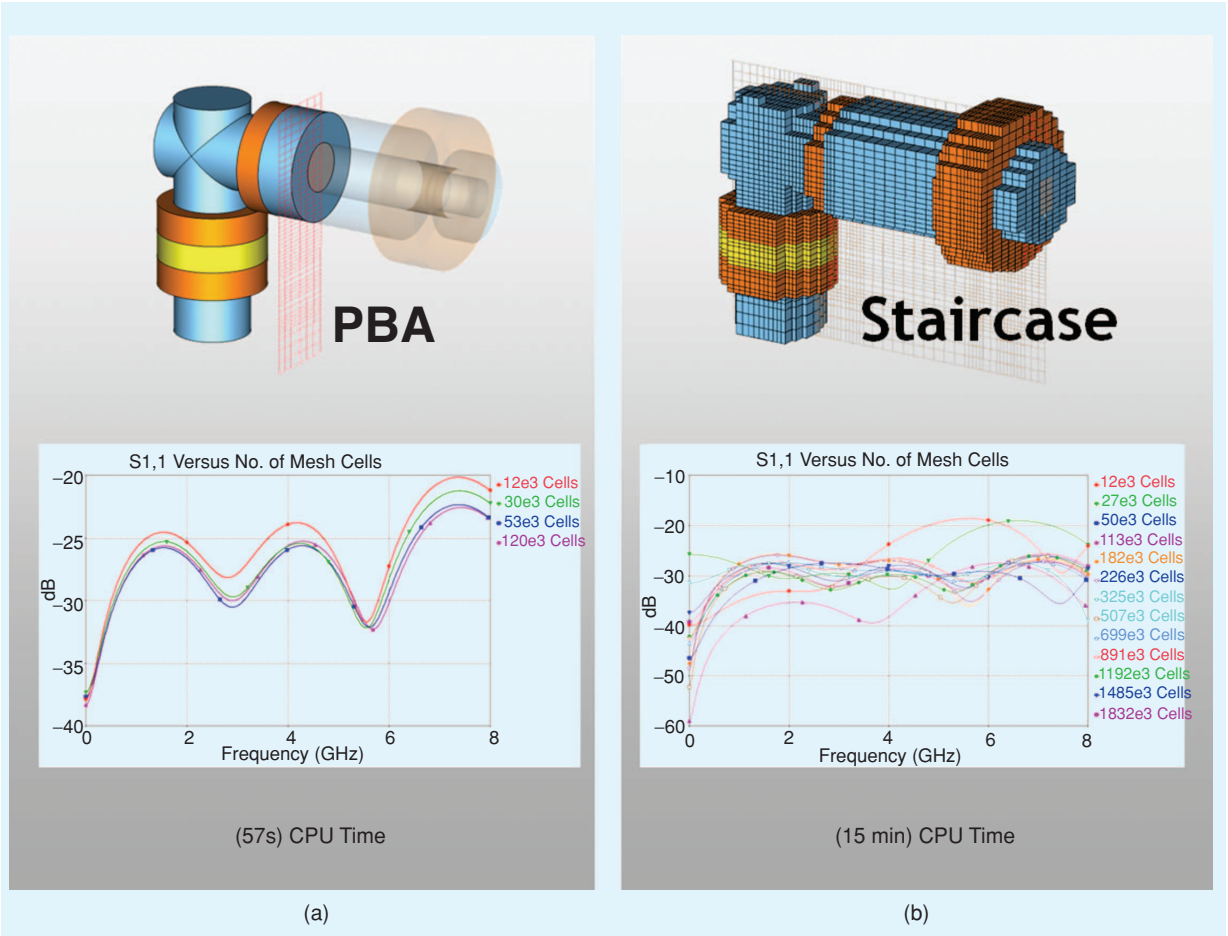


Figure 5. *Solution convergence for the connector example. When making the mesh finer and finer, the S-parameter results in the PBA case get closer and closer to the final solution. For the staircase mesh, the convergence is not as smooth as in the PBA case. It takes the staircase model 15 times longer on the same computer to reach the same convergence goal. For a comparison of the converged results, refer to Figure 3.*

in regions where small details are present. Additional exceleration of the simulation can be achieved by using different time steps at different mesh levels. Although many different subgridding algorithms have been proposed, many of them exhibit the so-called long time instability (see, e.g., [15] for references and an explanation of the phenomenon). The example in Figure 7 illustrates the impact of a mesh with hierarchical subgrids. It was solved with a subgridding algorithm with mathematically proven stability [16]. The computing time is reduced significantly by a factor of 9.5.

Frequency Domain

A characteristic of frequency domain solvers is the implicitness of this approach; the resulting system is typically a large linear system of equations. Thus, a matrix inversion is needed in order to obtain the solution for one frequency, no matter whether the grid is structured or not. In commercial applications, FEM on tetrahedral grids [12] is therefore the most popular general purpose numerical method. Tetrahedrons are the simplest volume entities, and their flexibility in approximating arbitrary geometries has many benefits. However tetrahedron quality is crucial: very flat tetrahedrons may compromise solution speed and accuracy as they make it more difficult for the algebraic solution method to solve the system.

There are two distinct methods of solving the linear systems of equations resulting from FEM discretization: direct and iterative solvers. A direct solver works directly on the system of equations derived from the discretization. Its key advantage is that it can solve for several port excitations at the same time in parallel. On the other hand, the memory requirements are quite high. Typically, the memory requirements increase quadratically with the number of tetrahedrons. Iterative solvers transfer the original system of equations into another one that can be solved by repeated application of operations according to the specific algorithm. The iterative algorithm has to be executed for each excitation individually. In compensation, the memory requirements are much less compared to a direct solver. Similarly to the time domain methods, where small time steps lead to many steps to be simulated, the overall computing time of a frequency domain method also depends, for both types of solvers, on the sampling granularity of the frequency range of interest.

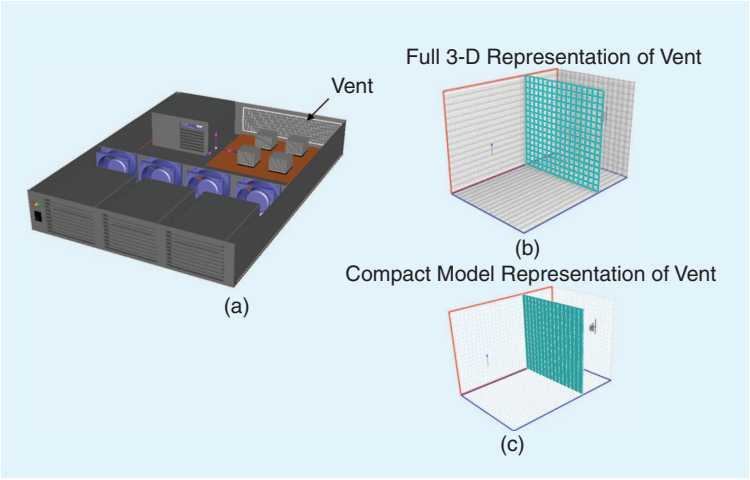


Figure 6. *(a) Compact model applied to a vent in a computer housing. Comparison of the mesh (b) for the full 3d structure and (c) for the compact model description. The use of a compact model can reduce the number of mesh cells significantly, in this example by a factor of 10.*

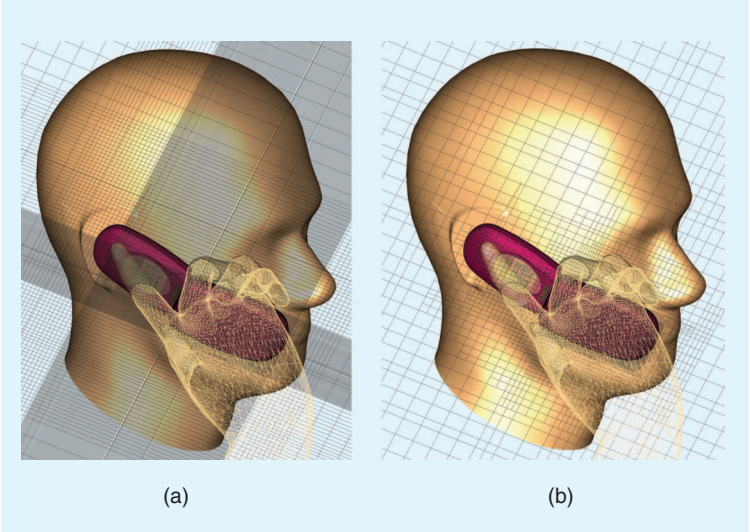


Figure 7. *Subgridding mechanisms reduce the number of mesh points in a simulation. In this example (a) the full grid is 20 times larger (35e6 mesh nodes) than (b) the subgridded version (1.75e6 mesh nodes).*

Frequency domain solvers are well suited to solve infinite periodic problems, such as phased arrays, frequency selective surfaces (FSS), photonic band gap structure (PBG), etc. Periodic boundaries can be set up either with a phase difference between them or, more practically, with a certain scan angle. A Floquet mode port is a useful addition to this capability. It enables the usage of plane waves to monitor polarization or RCS, as well as the determination of main and grating lobes of a phased array.

Special Filter Solvers—MOR and Modal Analysis

While frequency domain solvers are mostly well suited to tackle resonant problems, and some of them are especially suited for filter simulation. For example, a model order reduction (MOR) solver [17] works on both tetrahedral and hexahedral grids and can also use PBA. It does not calculate the EM fields, but directly accesses the

dominant modes of the matrix and introduces a reduced order replacement. In other words, it compresses the matrix to a much smaller size while keeping the information of interest in it. With this smaller system matrix, the S-parameters of the original device can be derived in an extremely short time. Where applicable, this approach may be 100 times faster than the others presented previously.

Another special approach is also particularly well suited for resonant devices. A modal analysis solver [18] calculates the eigenmodes of the device and uses them to interpolate fields in the interesting frequency range. Compared to a general purpose frequency domain method, this approach may be an order of magnitude faster.

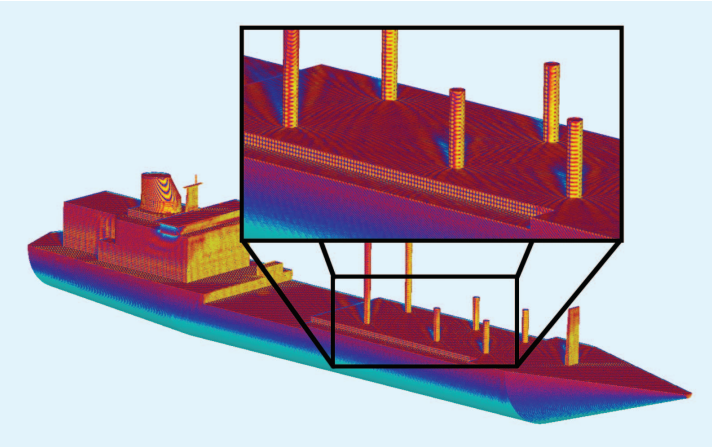


Figure 8. *Electrically large problems can often only be tackled with efficient integral methods such as MLFMM. The ship model is about 130 m long. It is illuminated with a plane wave at 1.5 GHz. The electrical size of the problem is therefore 650 wavelengths. Shown are the currents on the metallic surface.*

MoM-MLFMM

The MoM [13] only discretizes the surface of the devices rather than the entire volume. It shows advantages if the structure is predominantly metallic, electrically small, and preferably also small compared to the calculation domain, since the free space needs not to be modeled.

Typically, it is a very memory intensive method because the system matrix is not banded but fully populated. Since all these elements need to be stored, the range of practical application is typically limited to geometrically simple structures.

One important extension of the MoM is the multilevel fast multipole method (MLFMM) [19], which enables the simulation of electrically very large problems, such as the RCS of airplanes or antenna placement on ships (Figure 8). Using the same discretization as the MoM, this extension saves storage by grouping elements together. However, this method is only advantageous for very high frequencies.

Tips and Tricks

Probably the two most important questions that a user of a simulation tool is asking are:

- How accurate is my simulation?
- How long will it take to achieve an accurate solution?

To obtain an accurate solution after the simulation, there are quite a few ingredients:

- model the reality correctly
- ensure that the mesh is fine enough
- ensure that the solution of the discretized system of equations is numerically accurate.

Modeling the Reality

Excitations

For exciting the desired modes in the device, ports need to be defined at the locations at which, in reality, the sources will be connected. This is usually at some point along a transmission line (waveguide, microstrip, etc.).

A discrete port is simply a lumped voltage or current source, possibly with nonzero internal impedance/admittance. The source is connected by perfectly conducting wires to two points of the device [Figure 9(a)].

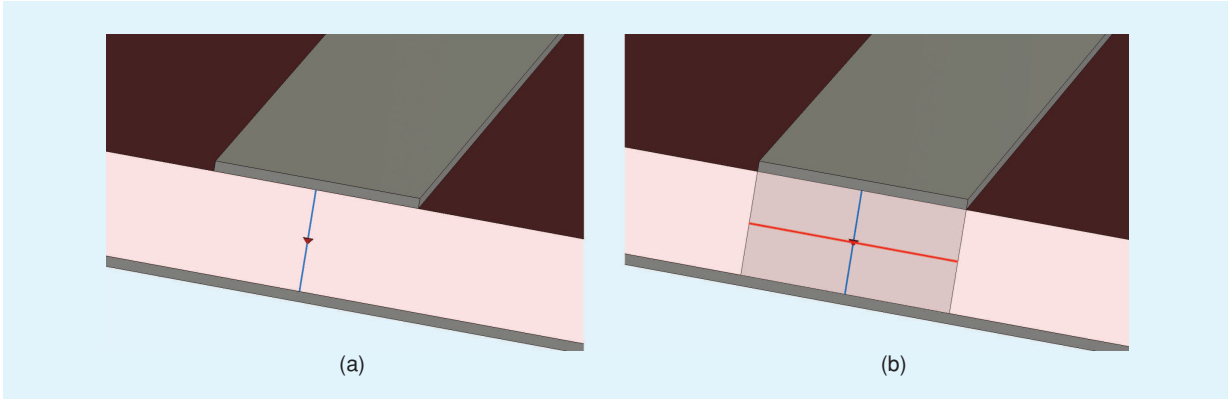


Figure 9. *(a) Discrete port: two wires with a source in the middle. (b) Face port: the source is distributed along the red line.*

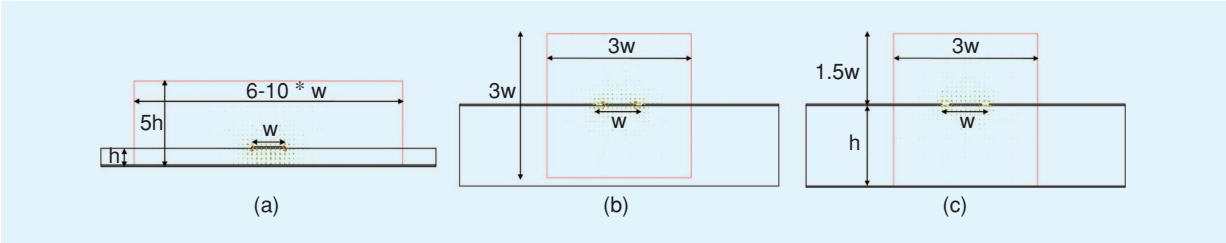


Figure 10. *Port size rules of thumb for: (a) microstrip, (b) ungrounded, and (c) grounded coplanar line.*

Long connection wires may strongly influence the solution. This is because of the wire inductance, which grows linearly with the wire length. To reduce the parasitic inductance of the discrete port, the so-called face port (or delta-gap port) has been proposed. Here, the voltage source is distributed along a small gap in a metallic face [Figure 9(b)]. The face port has a much smaller self inductance (imagine it as a parallel connection of many wire inductances).

The discrete or face ports will always introduce a small perturbation of the numerically calculated field at the location where they are placed in the model. To completely eliminate this perturbation, one can imagine extending the excited transmission line to infinity, thus preventing any reflections from appearing. Of course, no infinite structure can ever be modeled numerically, so a special type of port, the so-called waveguide port was introduced as a means of truncating the infinite line, without introducing any perturbations.

A waveguide port is a surface perpendicular to a transmission line on which the modes that can propagate along the transmission line are calculated. The field patterns corresponding to these modes are then used as excitation during the simulation. To ensure accurate mode calculation for arbitrary line configurations, the modes are typically calculated by solving a two-dimension eigenmode problem on the port's surface.

The size of the waveguide port is of utmost importance for the accuracy of the solution. Whereas for a hollow or coaxial waveguide the port size is clear—it should be as large as the waveguide's cross section—for other types of transmission lines (microstrip, stripline, etc.), the user might often have difficulty in guessing just how large the waveguide port should be. These transmission lines allow the propagation of static-type TEM or quasi-TEM modes, whose fields become zero, theoretically, at infinity. A few rules of thumb are given in Figure 10.

It is recommended, however, to make a few tests with the port size before starting the longer-lasting 3-D simulation. Just let the program calculate the port modes and have a look at the fields at the port, especially at the port's boundary. You should see no fields at the boundary. If there are fields at the boundary, the port size needs to be increased (Figure 11).

The first golden rule of an accurate simulation: never start the simulation before checking if the port modes are the expected ones!

Boundary Conditions

As already mentioned, the simulation domain, infinite in reality, has to be truncated for the purpose of simulating it on a computer. At the boundary, special boundary conditions need to be imposed, depending on the real operating conditions of the device.

For example, if the device that needs to be simulated is in reality placed within a metallic box, then electric boundary conditions (which impose zero tangential electric field, just as for a perfect metallic object) can be used on all sides of the boundary. An infinitely extended groundplane can be modeled by an electric boundary condition as well.

If the structure is placed in open space, such as an antenna, then a so-called radiation or absorbing boundary condition is the right one. It simulates the unperturbed propagation of EM waves through this boundary. When choosing the domain's truncation, do not forget to leave some free space around the antenna! A perfectly matched layer (PML) [21] boundary requires just a fraction of a wavelength of additional space,

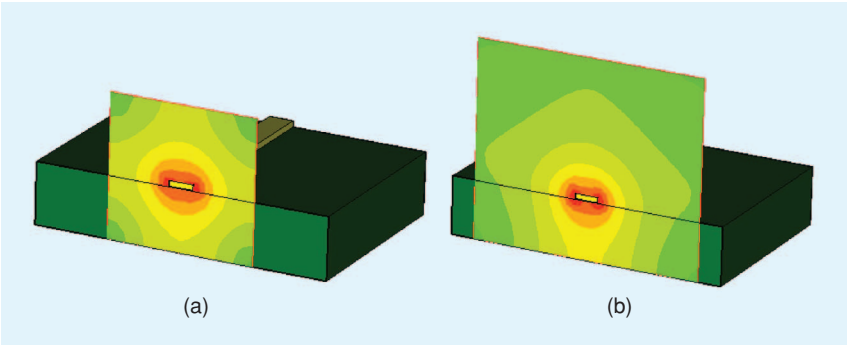


Figure 11. *Absolute value of the electric field (represented in logarithmic scale) at a microstrip port. (a) Port size is too small; electric field has considerable magnitude at port's border and will negatively impact on the solution's accuracy. (b) Port size has been increased laterally and above the microstrip and fields are practically zero (green colour) at port's border.*

whereas other absorbing boundary conditions often need more than one wavelength. Absorbing boundary conditions should be used only when necessary since they typically require more computing resources than, e.g., the electric ones.

For infinite periodic structures, the periodic boundary conditions are available. Whenever both the simulated structure and the excitation are symmetric, the usage of symmetry conditions can reduce the number of unknowns by half for each symmetry plane and therefore shorten the simulation time.

Material Properties

The permittivity, permeability, and conductivity values for all materials present in the model naturally play an important role in the solution's accuracy. Often, these values are frequency-dependent (dispersive materials), and the more accurately this frequency dependence is known, the more accurate the solution can be. Frequency-domain solvers, as well as the advanced time-domain simulators, can take this frequency dependence easily into account.

Please do not forget that the often used constant tangent delta material model is actually fiction. No material can have a constant loss tangent from dc to several GHz. Even the most common materials, such as Flame Retardant 4 (FR4), exhibit a more complicated dispersion—in the case of FR4 the first order Debye model appears to be sufficiently accurate.

Meshing the Structure

How fine does the mesh need to be? First, it should be fine enough to correctly represent the geometry. Second, it should be fine enough to represent the possibly sharp field variations within the device.

With most time-domain simulators, the used hexahedral mesh leads to a staircase representation of the boundaries, so the mesh needs to be made quite fine just to obtain a good representation of the geometry [Figure 12(a)]. The advanced conformal meshing eliminates this drawback by using the memory-efficient hexahedral mesh almost everywhere in the model and special algorithms conforming to the curved boundaries at material interfaces [Figure 12(b)]. This way, a considerable saving in terms of mesh cells can be achieved. Although tetrahedral meshes can, in principle, offer a good geometry approximation, this is only true if the real structure is meshed; some meshers require the segmentation of round structures and finally lead to polygonal approximation of curvatures [Figure 12(c)].

Representing the field variations in the mesh is an even more complicated issue. The first rule of thumb that can be applied a-priori, before any simulation is started, is that in a time-domain simulation with hexahedral mesh, the size of a mesh cell should never be larger than $\lambda/8$, where λ is the wavelength corresponding to the upper limit of the interesting frequency range. Mesh cell sizes of $\lambda/10$ or $\lambda/15$ are often successfully used in practice. For frequency domain FEM solvers based on second-order finite elements, $\lambda/4$ is a good value to start with. Of course, a model is typically made of several materials. Since the wavelength is dependent on the material properties, the size of every individual mesh cell depends on the material it is filled with. That is why programs that only allow a uniform mesh (the same mesh cell size everywhere) may lead to an unnecessarily large number of mesh cells.

For lossy materials, the rule of thumb is to ensure two to three mesh lines within the skin depth. This can prove disadvantageous for good conductors at high frequencies since the tiny skin depth would lead to tiny mesh cells and considerably increase the simulation time. Advanced simulators apply special surface impedance models for metals during the simulation process and eliminate completely the need to mesh the skin depth.

How about sharp field variations—field singularities—due to geometrical features, such as edges, corners, etc.? There are two ways to represent them in the mesh. The a-priori solution used by some field simulation programs is to automatically detect these features and to use advanced edge/corner correction algorithms during the simulation. A second way is increasing the mesh density

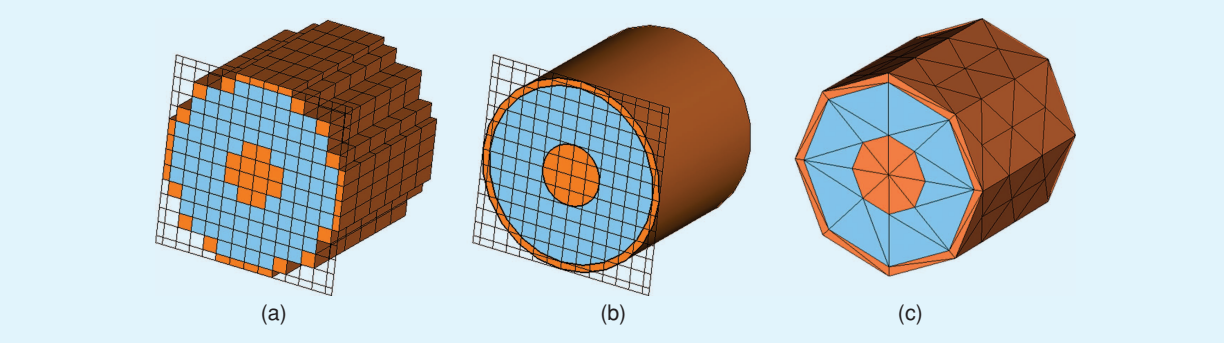


Figure 12. *Hexahedral and tetrahedral mesh for a piece of coaxial cable. (a) The staircase mesh provides a poor description of curved surfaces, unless a very fine mesh is used. (b) Conformal boundary approximation ensures the required geometric accuracy, with a minimum of mesh cells. (c) Tetrahedral mesh generators often require a segmentation of round structures, leading to a poor geometrical approximation.*

a-posteriori by the so-called adaptive meshing, which will be discussed later. These approaches are applicable in both time and frequency domain.

All this seems very complicated, and it appears almost impossible for a normal user to achieve a mesh of good quality. Don't worry, any advanced simulation program should be able to do all these steps for you: generate an initial mesh according to a minimal user input (e.g., number of steps per wavelength), taking into account geometry, material properties, and sharp corners and edges and refine the mesh through an automatic adaptive meshing, until convergence is reached.

With a minimum of user input however, the size of the final mesh can be optimized and thus reduce the overall computing time. For instance, you should ensure that there are at least two mesh cells within the substrate thickness, two to four mesh cells across a strip, and two mesh lines in a radiating gap (Figure 13). The mesh cells should be smaller close to metallic edges to sample the fringing fields. The height of the microstrip only has to be discretized if the used software does not support finite thickness metallization.

Accuracy

Accurate Numerical Solution

In frequency domain simulations, a linear system of equations needs to be solved at each frequency point. If the condition number of the system matrix is large, for example, because some tetrahedra in the mesh are excessively flat, the solution may be quite inaccurate. When using an iterative solver, a large number of iterations may be necessary.

In a time-domain simulation there is no system to solve. Issues like matrix conditioning number are irrelevant here. The main accuracy issue in the time domain simulation is related to the inverse Fourier transformation of the time signals, in order to obtain frequency-domain parameters. Namely, all signals should start at zero and end at zero in order to ensure accurate frequency-domain values. Especially for high-Q structures, the output time signals continue to oscillate a long time even after the excitation has been turned off (Figure 14). A good time-domain simulator will however provide the user automatically with a criterion on when to stop the simulation.

The position of a resonance will settle quite quickly and will be quite accurate even if the simulation is stopped too soon. The amplitude of the S-parameters however will only be accurate if the time signals have sufficiently decayed. To predict the correct amplitude, algorithms such as an autoregressive filter can applied on nondecayed signals and considerably save simulation time.

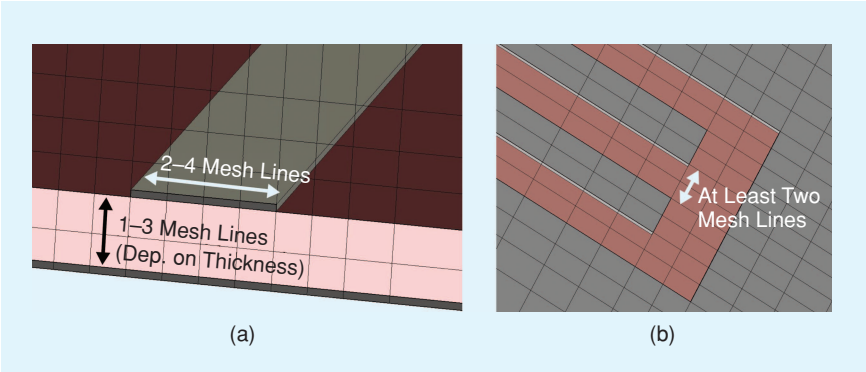


Figure 13. *Rules of thumb for meshing planar structures with hexahedral meshes (grey-metal, dusky pink-substrate). (a) Discretization of a microstrip. (b) Discretization of gaps inside a metal sheet.*

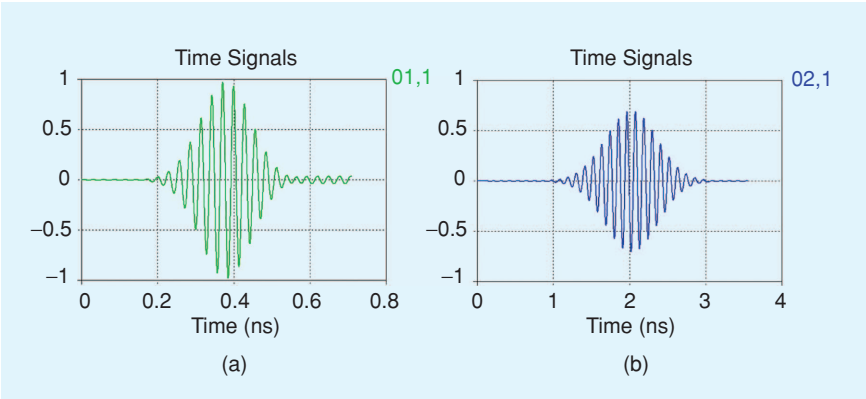


Figure 14. *Time signal examples. (a) The output signal still oscillates with a relatively high amplitude at the moment when the simulation was stopped. The frequency-domain results (e.g., S-parameters) are most likely inaccurate. (b) A time signal which is sufficiently decayed when the simulation is stopped will provide accurate frequency-domain results.*

Mesh Adaptation and Convergence

The accuracy of a simulation result has to be tested by performing a convergence study. In a convergence study the number of mesh cells is continuously increased until the results of interest, usually S-parameters, do not change anymore, at least not significantly. A convergence study is thus an essential part of any simulation project.

Many software tools feature automatic mesh adaptation schemes. Typically fields are evaluated after a simulation run. Wherever strong field variations occur, the

mesh is refined and the simulation is restarted. This process is repeated until the results do not change significantly anymore.

Although convergence study and mesh adaptation appear to be very similar approaches to guarantee accurate results, in practice they are different. For a convergence study, we assume that the geometry approximation of the structure as well as the results in the entire frequency range of interest are improved continuously with the refined mesh.

Frequency domain solvers perform the mesh adaptation typically only for one frequency, per default usually the highest frequency in the band of interest. The highest frequency is, for example for filters, not necessarily the one that is relevant for the device functionality. A relevant frequency has to be chosen for mesh adaptation. This information is reliably available only a posteriori. In addition, the field distribution might change significantly with frequency, e.g., for multiplexers or multiband antennas. One single adaptation frequency is not sufficient in such cases. Either the simulation has to be split up into several separate frequency bands, or several adaptations frequencies have to be used in one simulation over the entire band.

In order to derive accurate simulation results, the geometry representation on the grid has to be as good as possible. Particularly tetrahedral grid based frequency domain solvers do often not improve the geometry approximation during mesh adaptation. In the mesh adaptation process the initial tetrahedrons are simply subdivided in order to improve the field sampling (Figure 15). Therefore we see a convergence of results, though not for the input model but for the initially approximated geometry. This effect is even more critical if shapes are segmented before simulation (Figure 16).

In contrast to frequency domain, the time domain approaches can perform the mesh adaptation broadband. Moreover, every refinement also entails a better geometry approximation, since the entire meshing process is restarted at every mesh adaptation step.

Finally it should be mentioned that, unlike a tetrahedral mesh, a structured time domain grid can be easily controlled by the user, by manipulating mesh lines or meshing densities. Thus the final mesh of an adaptation is nearly reproducible by the user without rerunning the adaptation.

Checklist for accuracy

- Do the chosen ports correctly model the reality?
- Are the port modes and line impedances the expected ones?
- Are the material parameters the right ones on the whole frequency range?
- Is the mesh reasonable and fine enough?
- Have all output time signals decayed to almost zero in a time domain simulation?
- Was a convergence study performed?

And last but not least:

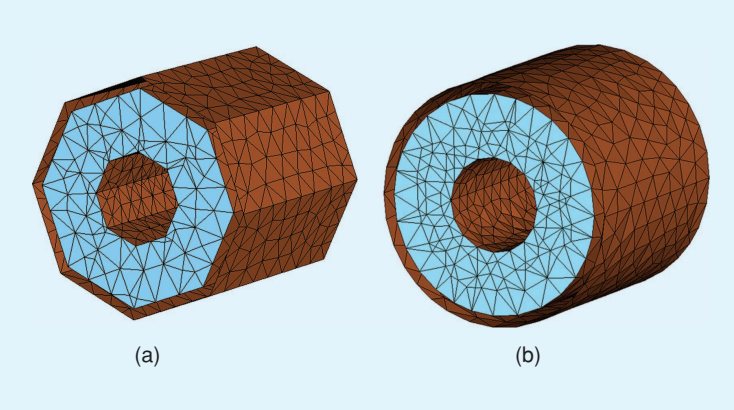


Figure 15. *Final mesh after the adaptation process for a piece of coaxial cable. (a) Mesh adaptation without snapping on the true geometry. (b) Snapping onto the geometry during the adaptation process leads to a good approximation of the geometry and hence to more accurate results.*

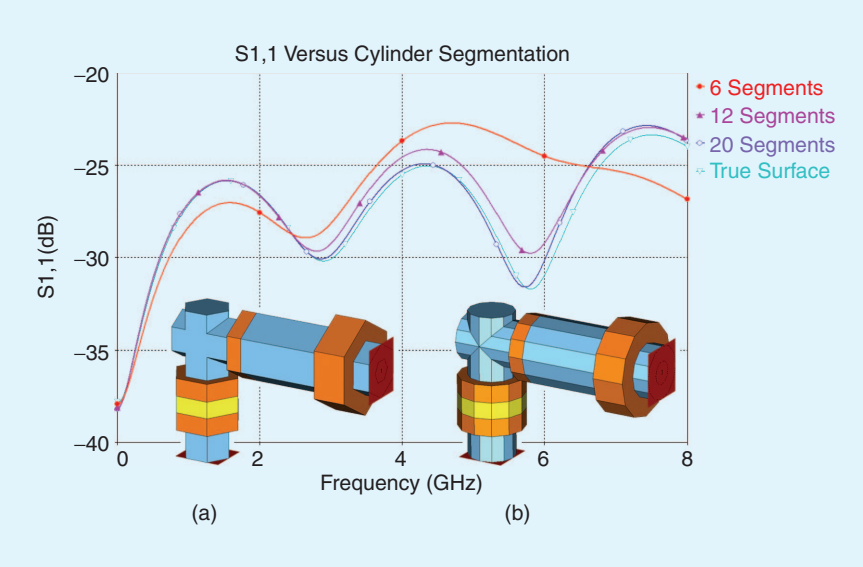


Figure 16. *Mesh adaptation and convergence. The cylinders of the connector model are segmented before meshing. The small connector pictures show the (a) 6 segment and the (b) 12 segment version. In all cases, a mesh adaptation was performed and the S-parameters were converged.*

- Is the model just as large or small as in reality? (mm instead of inch, a cable which is 3.2 mm long instead of 2.3 mm long, these things happen more often than one thinks!)

How Much Accuracy Do I Need?

The answer to this question depends on the purpose of the simulation, as well as on the phase in the design process. In the beginning, the design is probably still far from the sought optimum, and it does not make sense to look for an excessively accurate solution for a design variant that will most probably not be retained as final. You can set up the simulation with a coarse mesh and stop the simulation quite early.

Towards the end of the design process, when you are close to the design goal, it is worth investing more resources in a more accurate solution: make the mesh finer and allow the time signals to fully decay towards zero (in a time-domain simulation) or set the error criterion for the linear equation system to a lower value (in a frequency domain simulation).

The verification of measurements or analytic results requires the highest accuracy settings

Time Domain Versus Frequency Domain

As we have seen, the simulation process in time domain seems to be more complicated as far as S-parameters are concerned, but it has many advantages. Only one simulation is required for a broadband result. In addition we can benefit from an interesting property of the Fourier transform: the frequency resolution Δf of the spectrum relates to the signal length $t_{\max}$ in time domain by the Nyquist-Shannon theorem for limited-bandwidth signals $\Delta f = 1/(2t_{\max})$ [25]. Since at the end of a time-domain simulation all signals have, ideally, decayed to zero, we can prolong the signal by just adding zeros at the end in order to increase $t_{\max}$. This means that we can calculate the spectrum with an arbitrarily fine frequency resolution, and, most importantly, without additional computational effort. Unlike in frequency domain, in a transient simulation, it is thus virtually impossible to miss sharp resonances inside the requested spectral range.

In a time domain simulation, a signal has to enter and leave the device under test. Our connector does not have any resonances; it is supposed to behave like a broadband transmission line. Therefore, the simulation runs quickly. If there would be resonances, the transient signal would excite them and after the excitation signal has vanished, these resonances would continue to ring with their energy decaying according to the device's quality factor [Figure 14(a)]. The transient simulation can be terminated when a steady state is reached, or when the signal can be predicted by using digital signal processing techniques. Frequency domain solvers do not face this problem. To find the resonance frequency in high Q structures may require numerous simulations though.

Although the finite thickness of some metallization is technically relevant, it is usually not considered in most solvers. In FEM, its inclusion leads to a large number of tetrahedrons at the edges, or to tetrahedrons with a poor quality. In standard time domain methods, the thickness has to be sampled by a mesh cell. This will not lead to a large increase in mesh size. However, these cells will be very small, which will in turn reduce the time step because of the CFL criterion, and therefore increase the simulation time. Conformal methods such as FIT with PBA face no problem here, because the metallization thickness can be considered inside a mesh cell without compromising the time step. For thin dielectric sheets, similar efficient subcell models are available [26].

There is one other distinctive feature, the electric size. Generally, the discussed high-frequency solvers are effective for electric structure sizes within the range of about 1/1,000 to 1,000 wavelengths. The lower bound of this frequency range sees slight performance advantages for the general purpose frequency domain. Towards the upper bound the memory requirements become relevant.

On a typical workstation (8GB RAM) problem sizes of about 40 wavelengths in each spatial direction can be tackled with a transient solver, whereas FEM is restricted to about ten

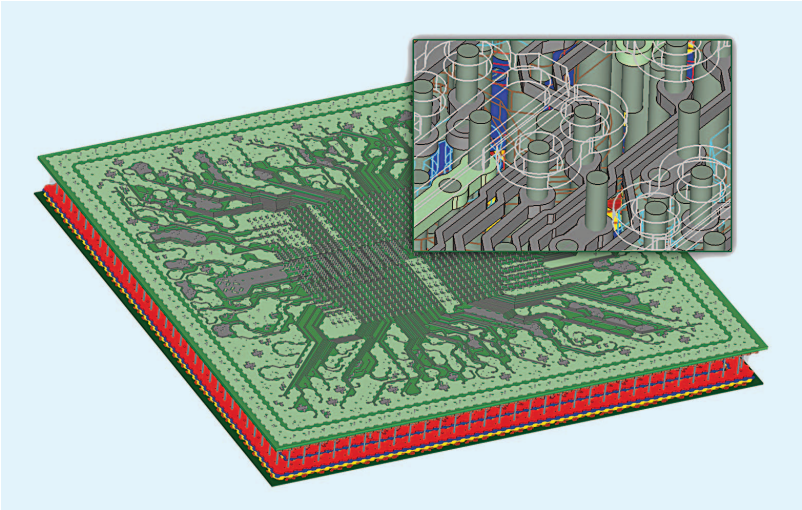


Figure 17. *A complete IBM package layout* [23] *used for full wave signal integrity analysis. It consists of eight metallization layers and 40,000 geometrical entities. The full package, shown here in total and detailed view, was imported into CST MWS for a full wave analysis. The benchmark fraction was solved by using the transient approach and the FD solver (27 million mesh nodes and 5.3 million tetrahedrons, respectively). The transient solver model of the full package had 640 million mesh cells and 3.7 billion of unknowns respectively* [24]. *This level of detail made the usage of the FD solver for a simulation of the full package unfeasible.*

wavelengths. Beyond these problem sizes, the use of an MLFMM solver is advisable since it is specifically designed to efficiently tackle electrically very large problems.

The lower memory requirements of the time domain methods allow also the solution of very detail rich structures (Figure 17). In the scope of this article we do not want to discuss what can be done on a hardware level, to extend simulation speed or accessible model sizes.

Conclusions

How can I select the best simulator? Most people would think it is obvious. Some will take the most accurate. Others will take the quickest, or the cheapest. All these selection criteria need to be looked at as a whole in order to make an informed choice. A good overall criterion would be something like the simulator's quality factor: Q = Accuracy/Effort.

Therefore, choose the program which gives you the best accuracy for a given simulation duration, or sum of money, or RAM, or all three together (= Effort) and you won't do anything wrong. Or, if it's accuracy that is of utmost importance, choose the program that achieves the desired accuracy with the least time and memory effort. By the way, do not forget about the labor costs while integrating the software into your design flow. A program with a good user interface and a high degree of automation will save valuable engineer's worktime and therefore money.

Beware of brute-force hardware arguments like "on a cluster, program X is also very quick." An intelligent algorithm is quick on any type of hardware and is even quicker on a faster computer, clusters or graphics acceleration card. It's the combination of intelligent algorithms and best available hardware that will give the user the optimal computing speed.

As we have seen, there is not one single solver approach best suited for all types of applications. It is very convenient if several solver types can be selected just from the one modeling interface. It would be even more convenient, if the software chose the best suited solver by itself.

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[29] All simulation pictures created with CST MICROWAVE STUDIO, except Figure 6, created with CST MICROSTRIPES.