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Introduction to Numerical Modeling

1.1 MODELING AS AN INTELLECTUAL ACTIVITY

Humans often attempt to understand physical phenomena by reduction to the familiar. At the end of the nineteenth century, scientists used models of electric and magnetic phenomena that were essentially mechanical in nature [1]. Mechanical phenomena at that time were accorded the status of familiar concepts and, by analogy to them, electric and magnetic phenomena were made plausible. Irrespective of their explanatory significance, it cannot be denied that models are very useful in several respects [2]. If the laws of a new phenomenon have the same form with those of another which has already been studied, then the consequences of the latter can be transferred to the new phenomena. This offers intellectual economy, strengthens the generality, and broadens the scope of our understanding of the world. A well chosen model facilitates the grasp of a new phenomenon and can be an effective heuristic tool in the search for explanations.

Numerical modeling is an activity distinct from computation. The endless printouts of numbers generated by computers are meaningless outside a system of knowledge and rationality that stems from human activity and experience. Numbers by themselves do not convey substantial information unless they can be used as evidence to justify or reject conceptual models of the phenomena we observe [3]. By repeated observations, we establish regularities which are embodied in models (mathematical or otherwise). This is a never-ending process which generates models of increasing generality and power. It is worth pointing out that however general and sophisticated a model is, it is never the real thing. Whether a perfect model is possible is a philosophical question of great

complexity. However, a pragmatic answer to this question can be given which may be acceptable for engineering models. A model that is “perfect” in the sense of being identical to the real thing will be of limited use to the engineer and therefore undesirable. It will be as unwieldy as the real thing and will obscure the insights that a simple but effective model can often provide. The development of engineering models must therefore be a task focused on simplicity and clarity. Models must be simple—but not simpler than they have to be. It therefore follows that a task equally important as the development of a model is the identification, in a qualitative and quantitative manner, of its limitations. A consequence of this approach is that several different models are necessary to describe what is the same thing. An example of this can be seen in the modeling of a human being [4]. In embarking on this task the following question must be asked: “What is the intended application of the model?” If the answer to this question is that it is intended for clothes fitting, then a simple wooden structure padded with straw is perfectly adequate. If, on the other hand, the model is to be used for studying the effect on humans of rapid acceleration and vibrations, then a structure made of springs and masses will be the most suitable model. Similarly, a model for determining the body’s electrostatic field distribution will need to contain a large amount of water to account for the basic constituent of the human body which, by virtue of its high dielectric permittivity, will affect strongly the field distribution. A model of humans that consists of resistors and capacitors is quite effective in predicting electrostatic charging and discharging. There is no way of saying that one of these models is a better model of a human, except in the sense that it is or may be developed into a more general model.

The above example helps to illustrate the great variety of models that can be constructed. We all have a multitude of mental models of which we may not be conscious at all times. It is simply impossible to have a rational view of the world without some models.

The reader may be persuaded by now of the importance of modeling in all human activities. However, modeling per se, as a field of study, is in its infancy, and there is simply a very wide scope for study and development of the modeling process.

Focusing now attention on numerical models, it is worth pointing out that implicit to every modeling activity are the following more or less distinct steps adapted from Reference [5].

- a) *Conceptualization*. This is the first step in the modeling mental process whereby observations are related to relevant physical principles. (For exam-

- ple, I release an apple and it falls. This must have something to do with gravity and not with its color!)
- b) *Formulation.* This step consists of the more detailed formulation of the physical ideas, perhaps in a mathematical form. (For example, in the example above, state Newton's Law $\mathbf{F} = m\mathbf{a}$ and quantify other factors that may be thought to be relevant, such as air drag, etc.)
 - c) *Numerical implementation.* During this stage, the mathematical or other model described above is prepared for solution—most probably by a digital computer. A solution algorithm is developed that is suitable for implementation by the computer. This process can be a simple one (as for the apple example) or very complex (as with most problems in electromagnetics).
 - d) *Computation.* This stage involves the coding of the solution algorithm using one of the computer languages and the development of preprocessing and postprocessing facilities. Large programs may involve extensive number crunching and press computing facilities to their limit. Issues of computational efficiency must be considered carefully at this stage.
 - e) *Validation.* Modeling complex problems involves a number of simplifications and approximations. At any stage during the process described above, unacceptable errors may be introduced. It is not uncommon for users of powerful models and computers to regard their output results as beyond reproach. It is, however, essential that results be checked for physical reasonableness. Confidence in models must always be tempered by an understanding of the complexity of real problems.

This brief introduction to modeling should convince the reader of the skill and sophistication necessary for good modeling. Conceptualizing demands the skills of a physicist and engineer to identify relevant mechanisms and thus develop the necessary framework for a solution. The more detailed formulation of the problem requires mathematical skills, as does the numerical analysis necessary for algorithm development and implementation. Computation can always benefit from the contributions of a computer scientist and engineer. Finally, the special gifts of an experimentalist are required to do critical, well documented experiments with the required accuracy and to interpret results for comparison with simulations.

Naturally, no single person can claim mastery of all these fields. Nevertheless, anyone seriously involved in modeling should aim to develop the skills, maturity, and confidence necessary to function creatively and efficiently in this exciting discipline.

In this text, which is focused on a single modeling method, it is not possible to present in detail all aspects of modeling. However, by a systematic approach to model building in *transmission line modeling* (TLM),

the basic processes inherent in many similar methods will be presented, and it is hoped that they will be of value in other applications and disciplines. The plan of the book is outlined below.

A general classification of modeling methods is given in the next section, based on the manner in which the problem is formulated. The chapter concludes with a section that aims to put TLM into context rather than offering a complete coverage of other methods.

The basic building blocks in TLM are electric circuit components and, more specifically, transmission line segments. The next two chapters give an introduction to the basic modeling philosophy and to standard transmission line theory. Subsequent chapters introduce model building from the simplest lumped components to the most general field distributions in three dimensions. The standard theory is presented in terms of application to electromagnetics. This avoids unnecessary complexity and loss of focus during the development of the basic concepts and techniques. Generalization to other applications (e.g., thermal, mechanical, etc.) is then straightforward and is presented mainly in Chapters 7 and 8. Applications and more advanced topics are presented in Chapters 9 and 10.

1.2 CLASSIFICATION OF NUMERICAL METHODS

Engineering models are used to establish a relationship between the input (source, stimulus) to a system and the output (response) from the system. This is shown schematically in Fig. 1.1. The process of Conceptualizing and formulation leads to the expression of the physical laws describing the system in a form of the type:

$$\mathcal{L}(\Phi) = \alpha \quad (1.1)$$

where

\mathcal{L} = a mathematical operator

Φ = a field function that must be determined

α = a source function

Basic classification schemes for numerical methods can be arrived at by examining the nature of Equation (1.1).

One criterion for classification is the domain in which the operator, the field, and source functions are defined. If these are defined in the time-domain, then the method is described as a time-domain (TD) method.

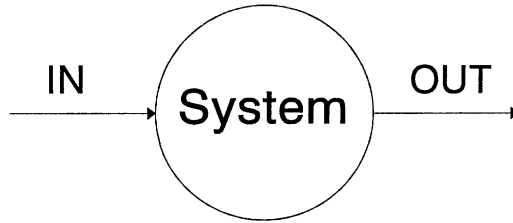


Fig. 1.1 Input/output in a system

Alternatively, the frequency domain may be chosen, leading to frequency-domain (FD) methods. Examples of the two formulations for the circuit shown in Fig. 1.2 are:

$$V_0 \cos \omega t = i(t) R + L \frac{di(t)}{dt}$$

for TD formulation and

$$V_0 = \bar{I} (R + j\omega L)$$

for FD formulation, where \bar{I} represents the current phasor.

Clearly, the TD formulation is suitable for studying transients and nonlinear phenomena, while the FD formulation is straightforward for studying the steady-state response to a sinusoidal excitation. In the TD, the function fully characterizing the system is its impulse response $h(t)$, while in the FD, the frequency response $H(j\omega)$ offers a complete system description. Since $h(t)$ and $H(j\omega)$ form a Fourier transform pair, any information available in the TD can be converted into the FD, and vice-versa. However, although the two descriptions are formally equivalent, issues of efficiency normally dictate which approach is the most convenient in a particular problem. For example, if the steady-state response at a single frequency is required, the natural choice must be a FD method. For tran-

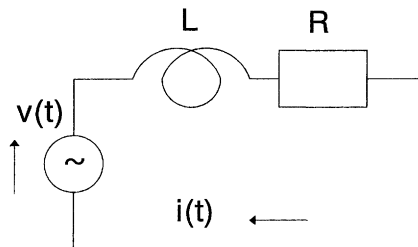


Fig. 1.2 A simple circuit used to demonstrate frequency- and time-domain formulations

sients, or when the response over a wide frequency range is required, a TD method may be the most appropriate.

For the simple example shown in Fig. 1.2, both “transfer functions” $h(t)$ and $H(j\omega)$ can be readily obtained in an analytical form. However, in most practical problems, the transfer function is a multivariable, multidimensional, discrete function defined over a large number of mesh points. It occupies a large amount of computer memory, and its determination and manipulation forms the formal task of solving a problem by numerical simulation.

Another criterion for classification is the nature of the operator \mathcal{L} used in Equation (1.1). It may be expressed in a differential or in an integral form, thus resulting into differential (DE) and integral (IE) numerical modeling methods, respectively. An example of differential and integral formulations of the same basic physical ideas can be seen in Gauss’s Law:

$$\nabla \cdot \mathbf{D} = \rho$$

$$\int_S \mathbf{D} \cdot d\mathbf{S} = Q$$

The former equation is a differential formulation and must be enforced at every point in the problem space. The latter is an integral formulation and must be enforced on surfaces in the problem space. Numerical methods fall broadly within these two categories.

A further class of methods, with its own special characteristics, is that of ray methods, which are based on concepts borrowed from optics. Several formulations are also available combining more than one method, and these are described as hybrid numerical methods.

In formulating a problem for solution by digital computer, the convenient concepts used in analytical techniques of infinitesimally small time and space steps (dt and dx , respectively) must be replaced by small but finite steps (Δt and Δx , respectively). This is fundamental in computer simulation because, if time-steps were infinitesimally small, a computer with a finite clock speed would require an infinitely long time to do the simplest calculation. Similarly, an infinitesimally small space-step would require a computer with an infinite number of memory locations. Therefore, implicit in every numerical simulation is the construction of a grid or mesh of points, covering the entire problem space, on which the relevant physical laws are enforced at successive time steps. It is arguable that at the atomic level physical processes are finite. However, in most practi-

cal simulations, the replacement of the concept of a continuum by the discrete approach is dictated by practical considerations, such as computer storage and run-time. Discretization in time and space therefore introduces errors that must be quantified and controlled in every numerical simulation.

In a differential method, the entire space has to be discretized, and this normally results in large computational requirements. In practice, if a suitable physical outer boundary surface does not exist in the problem (such as in the case of open-boundary problems), then an artificial “numerical boundary” must be defined to contain the computation within manageable limits. Defining the correct boundary conditions on numerical boundaries is not an easy task. On the positive side, the enforcement of physical laws on all points in space means that fine features, irregular shapes, and material inhomogeneities can be easily dealt with. In addition, in spite of the large number of quantities to be determined on grid points in space, the resulting equations can be solved relatively easily.

In contrast, in an integral method, physical laws are enforced on grid points lying on important surfaces of the problems and, hence, the number of quantities to be determined is smaller. However, the equations to be solved are usually more complex, so a relatively small number of points can be handled. Open-boundary problems can be dealt with rigorously in IE formulations.

This brief outline of DE and IE methods indicates that each general class has its own advantages and disadvantages, and that the best method is application dependent. A more detailed discussion of numerical methods may be found in [5].

The need for discretization in numerical simulation leads to the question of the choice of appropriate time- and space-steps. An answer to this question cannot be given without reference to the method used, errors, and application requirements. However, a useful practical rule is to choose a space discretization length that is smaller than one-tenth of the smallest wavelength of interest. For both classes of finite methods (DE and IE), and with computing facilities commonly available, it is difficult to envisage solving problems in three dimensions which are larger in physical size than a few wavelengths. At very high frequencies, it is advantageous to use ray methods. These methods can be applied when the wavelength λ is much smaller than the size of the features being modeled. Fields are calculated by taking into account reflected and diffracted rays. Methods based on geometrical optics (GO), the geometrical theory of diffraction (GTD), and other more general approaches are available.

1.3 ELECTRICAL CIRCUIT ANALOGS OF PHYSICAL SYSTEMS

It is undoubtedly true that humans model best when they use a medium with which they are familiar. Mechanical phenomena are closest to human experience and the first to be understood and formulated in scientific terms. The field of mechanics has long been understood in terms of a coherent self-consistent set of scientific principles. It was therefore natural that, during the beginnings of electrical science, mechanical models were used to aid understanding and make predictions. Electrical science now has the status of a well established scientific theory, and it therefore can be used as a model for studying other phenomena. While mathematicians are familiar with differential equations, electrical and electronic engineers have an intuitive understanding of how electrical circuits work and the significance of each circuit component. They are, therefore, more comfortable with circuit models than with the more abstract mathematical models normally used to study electromagnetic fields. Circuit models can also be used to study thermal and mechanical phenomena—an interesting development, considering the situation at the turn of the century. The purpose of this book is to provide a systematic treatment of the modeling process based on electrical circuit analogs. In this chapter, however, only a general introduction will be given. The modeling principles will be outlined with a broad brush to assist the reader in following more comfortably the detailed treatment in subsequent chapters.

The idea of using electrical circuits to model fields is not new. More recently, the work of Kron and others signposted the equivalence between field and circuit ideas [6–8]. However, no substantial progress could be made in exploiting these ideas, because the circuit models could not be solved using the calculation tools available at the time. Further development had to wait for the introduction of modern digital computers and the pioneering work of Johns and Beurle [9], which provided sufficient impetus for a rapid advance.

The analogy between circuits and fields can be understood by considering the transmission line circuit shown in Fig. 1.3. The voltage v and current i on the line are functions of time t and distance x . Kirchhoff's voltage (KVL) and current (KCL) laws on the lines give:

$$-\frac{\partial v}{\partial x}\Delta x = L \frac{\partial i}{\partial t} \quad (1.2)$$

$$-\frac{\partial i}{\partial x}\Delta x = C \frac{\partial v}{\partial t} + \frac{v}{R} \quad (1.3)$$

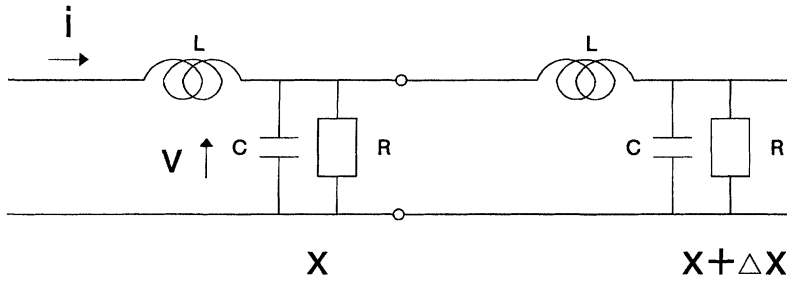


Fig. 1.3 A simple transmission line network

These expressions are strictly correct provided that $\Delta x \rightarrow 0$. Equations (1.2) and (1.3) may be manipulated to eliminate v and thus provide an equation containing i only:

$$\frac{\partial^2 i}{\partial x^2} = \frac{LC}{(\Delta x)^2} \frac{\partial^2 i}{\partial t^2} + \frac{L}{(\Delta x)^2 R} \frac{\partial i}{\partial t} \tag{1.4}$$

It can also be shown that in a one-dimensional EM field problem, the current density j is determined by the following equation [10]:

$$\frac{\partial^2 j}{\partial x^2} = \mu\epsilon \frac{\partial^2 j}{\partial t^2} + \mu\sigma \frac{\partial j}{\partial t} \tag{1.5}$$

where μ , ϵ , and σ are the magnetic permeability, electric permittivity, and electrical conductivity of the medium.

Field components E , B are also described by equations similar to Equation (1.5), which is known as the wave equation in a lossy medium. The analogy between the circuit [Equation (1.4)] and field [Equation (1.5)] problems is based on the similar form of these two equations. Similarly, analogues of Equations (1.4) and (1.5) may be found in three-dimensional problems, as shown in Chapter 6. The laws governing circuit behavior have the same syntactical structure as those governing field behavior. The isomorphism between Equations (1.4) and (1.5) means that the behavior of fields may be understood by studying the behavior of circuits. For the particular example considered here, the equivalence between circuits and fields is summarized in Table 1.1.

It is worth considering further the nature of Equation (1.5). Assuming a harmonic variation for j , i.e., $j(x, t) = j_0 \cos(\omega t - \beta x)$, the two terms on the right-hand side of this equation can be evaluated and their

Table 1.1 Equivalence between circuits and fields

<i>Circuit</i>		<i>EM Field</i>
i	\Leftrightarrow	j
$L/\Delta x$	\Leftrightarrow	μ
$C/\Delta x$	\Leftrightarrow	ϵ
$1/R\Delta x$	\Leftrightarrow	σ

magnitudes compared. The first term describes wave-like behavior, and given that $\partial j/\partial t \sim \omega j$, and $\partial^2 j/\partial t^2 \sim \omega^2 j$,

$$|\text{wave term}| \sim \mu \epsilon \omega^2$$

The second term describes diffusion-like behavior, and its magnitude is

$$|\text{diffusion term}| \sim \mu \sigma \omega$$

Hence,

$$\frac{|\text{wave term}|}{|\text{diffusion term}|} = \frac{\omega \epsilon}{\sigma}$$

In cases where $\omega \epsilon \gg \sigma$, wave behavior dominates. This is the case with propagation in air and low-loss dielectrics at high frequencies. When $\omega \epsilon < \sigma$, diffusion behavior prevails, as in propagation at low frequencies in lossy media. The circuit equation (1.4) thus can be used to model waves, diffusion, and any combination of the two. To model diffusion, the first term on the left-hand side of this equation must be negligible compared to the second. The diffusion-dominated equation (1.4) can then be used to model thermal conduction in a material. In this case, the temperature distribution $\theta(x,t)$ is determined by the diffusion equation:

$$\frac{\partial^2 \theta}{\partial x^2} = \frac{S}{k_{th}} \frac{\partial \theta}{\partial t} \quad (1.6)$$

where

S = the specific heat in J/Km^3

k_{th} = the thermal conductivity in W/Km

Clearly, the analogy between Equation (1.6) and the diffusion-dominated Equation (1.4) requires the equivalence shown in Table 1.2.

Table 1.2 Circuit and thermal equivalence

<i>Circuit</i>		<i>Thermal</i>
$\frac{L}{\Delta x}$	\Leftrightarrow	S
$R \cdot \Delta x$	\Leftrightarrow	k_{th}

Other circuits can also be used to model thermal problems, as will be discussed in more detail further in this book. The purpose of the previous brief treatment is merely to illustrate the principles of establishing analogies between different physical problems.

The circuit analogs described above would be of only educational value if their solution could not be found in a relatively simple manner. In engineering practice, it is important to develop models that clearly illustrate the important physical interaction, but a solution of these models is also necessary to predict behavior and optimize designs. Circuit models such as the one shown in Fig. 1.3 can be very complex in practice, especially when they are generalized to describe two- and three-dimensional distributions, as it will be shown later.

TLM provides a systematic, elegant, and efficient procedure for solving these networks. It is based on using transmission line elements to describe all energy storage elements. It is therefore important to summarize (see Chapter 2) aspects of transmission line theory that are important in understanding the implementation of TLM.

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