

Chapter 2

Numerical Simulation of Wave Propagation

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Abstract Wave equations are hyperbolic partial differential equations (PDEs) which describe the propagation of various types of waves, such as acoustic, elastic, and electromagnetic waves. In order to solve PDEs, the finite element method (FEM) can be used. After a brief introduction to the mathematical method used by FEM to evaluate the solution in nodes, where the polynomial curve that interpolates the differential equation has to be solved, we will describe the methodology used to solve the wave propagation problem described by the Helmholtz's equation. The wave propagation problem is analyzed by following specific steps: construction of the geometry to study, application of the boundary conditions, and meshing of the domain to be solved. The same procedure is used to simulate the behavior of piezoelectric transducers and the problem of wave propagation in medium with defects. Finally, the procedure followed for the simulation of acoustic problems using a specific software, i.e., COMSOL Multiphysics, is illustrated.

2.1 Introduction

The numerical simulation is commonly considered a mandatory passage in synthesizing a nondestructive testing (NDT) diagnostic system. Indeed, a number of design parameters need to be set on the basis of the response of the diagnostic system in different scenarios, which would be hardly reproducible in real physical setup. Whichever numerical tool is used to simulate the real system, it has to guarantee reliability, convergence, and possibly, a limited computational cost. The problem can be approached by using several different methods, such as analytical, finite difference, moment, finite element, and Monte Carlo, each having its strong and weak points. Among these, finite element method (FEM) has the advantage of combining good

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model precision with a typical easiness of use. Furthermore, it allows for tuning the degree of precision on the simulation domain on the basis of the specific requirements. This aspect is crucial in our application, because in general, the object to detect consists of a discontinuity of the propagating mean.

The FEM, such as the finite difference method (FDM), is a numerical technique designed to seek approximate solutions of problems described by a system of partial differential equations (PDEs), reducing them to a system of algebraic equations [4]. With this method, it is possible to solve problems whose analytical models described by a system of differential equations cannot be solved analytically. To this aim, the problem is discretized by subdividing the domain in a proper number of elements (from which the name of the method), then the solution is found only in specific points of those elements (nodes), and finally, a continuous solution is obtained by interpolating the solution on the nodes. The possibility to entrust the solution of the problem to a computer represents a great advantage. The more the discretization is fine, namely the more the elements are small, the more the FEM model is precise but also computationally costly. Therefore, dealing with such method requires to find the best compromise between such two conflicting issues, by taking into account the resources on hand.

This chapter is organized as follows. First, a general formulation of the FEM is given. Then the method is described in more detail for the case of a wave propagation problem. A specific paragraph is devoted to the study of the behavior of transducers, whose function is the conversion of the electrical signal into pressure waves and vice versa. After that, the problem of detecting defects into a mean by means of ultrasonic waves is described in depth. Appendix reports a tutorial for the development of a model of NDT ultrasonic system.

2.2 The Finite Elements Method

The first thing one has to define in using the FEM is the domain of the problem. After that, the state variables of the problem have to be defined. The domain is delimited by a boundary, except for the cases where it could be useful considering an unlimited domain; in such cases, particular elements are adopted, but this is not a case of interest for the scope of this book.

As for the continuous differential problems, the boundary conditions have to be defined in order to solve the problem. The boundary is subdivided into two parts that are characterized by a specific boundary condition. The nature of this condition depends on the physics of the problem, but in general, we can distinguish between boundary conditions where the value of the state variable is given (Dirichlet conditions) and that where the normal derivative of the state variable is given (Neumann conditions). Corresponding to such distinction, we can subdivide the whole boundary of the domain into a Dirichlet and a Neumann boundary, respectively.

The problem at hand in the FEM is first expressed in the so-called strong form and then it is translated in the weak or variational form to be solved. The first one

can be formalized in general as follows:

$$\begin{aligned} L\Phi &= g & \text{in } \Omega \\ \Phi &= g_0 & \text{in } \Gamma_D \\ \partial_n \Phi &= g_1 & \text{in } \Gamma_N \end{aligned} \quad (2.1)$$

where L is a differential (integral) operator, Φ is the state variable, Ω is the domain, g , g_0 , and g_1 are known functions, Γ is the boundary of the domain, which is subdivided into the Dirichlet boundary Γ_D and Neumann boundary Γ_N , and finally, ∂_n denotes the derivative of the state variable in the direction normal to Γ .

It is often possible to replace the problem of integrating the equations in (2.1) by an equivalent minimization problem. Problems like these are called variational problems and the methods which allow one to reduce the original problem in variational form are called variational methods. Such methods represent a common basis for different kind of analyses, among which, the FEM is included [12, 13, 22].

The first step to apply the variational methods consists of finding the functional of the problem, which is the function having a minimum in correspondence of the solution of the original problem [9]. This function is commonly called energy function W due to the fact that, like in nature, the systems spontaneously evolve toward states of minimal energy, but in most cases where the problem at hand is physical, the functional is actually an energy function, so that searching the solution of the system just corresponds to find a state of minimal energy.

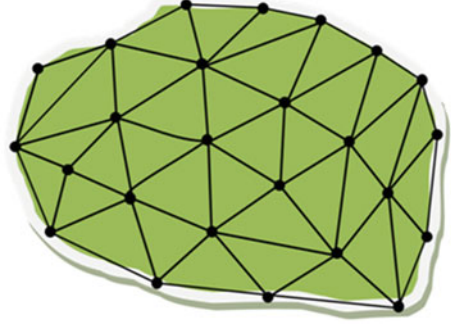
Generally speaking, the application of the FEM involves the following steps:

1. Discretize the domain of application of the differential equation as function of physical magnitude of field quantity V in a finite number of elements.
2. Define the governing algebraic equations as a function of field quantity V for a generic element.
3. Assembling of all elements in the solution region and determination of the total energy W , associated with the assembly of the elements expressed as a function of the values that the field quantity V assumes in each of the n nodes of the mesh: $W = f(V_1, V_2, V_3, \dots, V_n)$.
4. Solving the system of linear equations resulting from the application of the variational principle, by imposing the condition of minimum energy stored, equivalent to the equilibrium condition of the system. Thus, we require that the partial derivatives of the energy function W with respect to each nodal value of the potential are zero i.e.,: $\partial W / \partial V_k = 0$; $k = 1, 2, \dots, n$.

So we get a system of n algebraic equations whose unknowns are values that the field quantity V assumes in the nodes of the mesh, except for the nodes on the boundary of the domain, in which the magnitude (*Dirichlet conditions*) or the normal derivative (*Neumann conditions*) of the field quantity are known.

Therefore, the FEM is based on the discretization of the domain into elements. Without loss of generality, we can assume that the domain at hand is 2D and that the elements we have chosen are triangular. The value of the field quantity at any point inside of the generic triangular element will be determined by interpolating the values of the field quantity in the nodes of the corresponding element (Fig. 2.1).

Fig. 2.1 Discretization of the domain by means of triangular elements



The triangular elements are those that fill better the surfaces of the most varied forms. Actually, the elements with the minimum number of facets (simplex: segments in R^1 , triangles in R^2 , and tetrahedrons in R^3) are the most commonly used as default-element for the mesh by commercial softwares. The elements have a certain number of nodes, which in the simplest case, coincide with the vertices of the element. The FEM solves Eq. (2.1) only on the nodes of the mesh rather than on the whole domain, while the solution within the element is expressed in function of such nodal values. The relationship among the values of the nodes and the other points of the element is fixed a priori, so that in general, it does not fit exactly the actual values of the function. This relationship is called shape function and in general can be fixed arbitrarily, but for simplicity, it is often preferred to have a great number of elements and for each element a limited number of degrees of freedom. This is the reason why the most common choice is to assume linear shape functions.

We seek an approximation of the function $V(x, y)$ in the whole domain as the sum of the function within the elements $V_e(x, y)$:

$$V(x, y) \cong \sum_{e=1}^N V_e(x, y) \quad (2.2)$$

where N is the number of elements and

$$V_e(x, y) = a + bx + cy \quad (2.3)$$

is an interpolating linear function which gives the approximation within the element. More in general, the number of nodes could be much greater so that the interpolating function could be different.

For the convergence of the solution, the approximating polynomial has to satisfy the compatibility and completeness criteria [11]. This means that considering, for example, 2D elements:

- the functions (2.3) have to be continuous at element interfaces, i.e., along element interfaces, we must have continuity of V as well as continuity of the derivative of V normal to the interface;

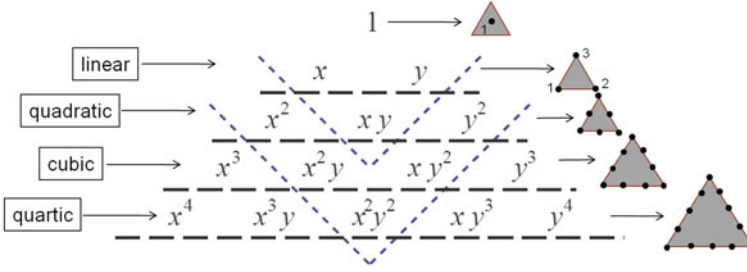


Fig. 2.2 Pascal's triangle (2D case)

- if the size of the elements tends to zero, the function (2.3) and its gradient must be constant within the element.

Furthermore, the approximating polynomial should be isotropic, i.e., the approximating polynomials should remain unchanged under a linear transformation from one Cartesian coordinate system to another. This is achieved if the components of the approximating polynomial are complete or, if incomplete, they are symmetric with respect to the independent variables.

In order to correctly select the terms of the polynomials, we can use the Pascal's triangle (see Fig. 2.2).

Assuming a linear interpolation within the elements implies that a proper size of elements (*mesh*) has to be considered in order to avoid introducing too coarse approximations.

The three coefficients in (2.3) are related to the value of the V_e in the nodes:

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}^{-1} \begin{bmatrix} V_{e1} \\ V_{e2} \\ V_{e3} \end{bmatrix}. \quad (2.4)$$

The coefficients obtained by Eq. (2.4) can be substituted in Eq. (2.3), obtaining at the end the linear function within the element, given by:

$$V_e(x, y) = \sum_{i=1}^3 \alpha_i(x, y) V_{ei} \quad (2.5)$$

that is, it is given by a linear combination of three functions, one for each node, where the weights are values of the V_e in correspondence of the nodes. The functions $\alpha_i(x, y)$ are called shape functions and, due to the initial choice, are linear.

As said before, a functional has to be defined to solve the problem [9]. The precise form of such functional depends on the form of the equation which describes the problem.

To fix the ideas, let us consider the case of a problem described by the Laplace's equation:

$$\nabla^2 V = 0. \quad (2.6)$$

The corresponding functional evaluated for the single element has the following form:

$$W_e = \frac{1}{2} \int |\nabla V_e|^2 dS. \quad (2.7)$$

The gradient of V can be expressed by means of Eq. (2.8):

$$\nabla V_e = \sum_{i=1}^3 V_{ei} \cdot \alpha_i \quad (2.8)$$

which can be substituted in Eq. (2.7), to give

$$W_e = \frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 V_{ei} \left[\int \nabla \alpha_i \nabla \alpha_j dS \right] V_{ej}. \quad (2.9)$$

Let us indicate the term in brackets with the notation C_{ij} . With this, Eq. (2.9) can be rewritten in matrix form:

$$W_e = \frac{1}{2} V_e^T [C_e] V_e. \quad (2.10)$$

The terms C_{ij} are obtained by combining gradients of linear functions, so they are constant and depend only on the coordinates of the elements nodes.

The complete functional to minimize is obtained by summing Eq. (2.10) for all the elements, as

$$W = \sum_{e=1}^N W_e = \frac{1}{2} V^T [C] V. \quad (2.11)$$

In Eq. (2.11), the variable vector V comprises the function calculated in all the nodes of the domain. As the same node belongs to more than one element, the matrix $[C]$ will not be concentrated around the diagonal, but in general, any entry could be different from zero. The definitive distribution of the elements of $[C]$ will depend on the order according to which they are considered and it is arbitrary, but the computational cost of minimization depends on such distribution. The minimum of Eq. (2.11) can be found by imposing the gradient to be equal to zero. Not all the values of V at nodes are variable. Indeed, the boundary conditions have to be fulfilled according to the formulation of the problem. As a consequence, the equations' system that gives us the minimum will be a nonhomogeneous system. Indeed, the terms of W that are the product between a variable and a fixed value in the derivation give rise to constant terms.

The minimum of the solution can be found by solving a linear equations' system:

$$[C_{\text{free}}]V_{\text{free}} = [C_{\text{bound}}]V_{\text{bound}} \quad (2.12)$$

where V_{free} is the vector of the variable values of the function and C_{free} is the corresponding coefficient matrix, while V_{bound} is the vector of values at the boundary of the domain and C_{bound} is the corresponding matrix of coefficients.

The number of nodes needs to be higher in the regions where the field variable has strong gradients. In these regions, in order to apply the method preserving the required accuracy, it may be necessary to thicken the nodes. The FEM allows to do that. Solving the system (2.12) is in general troublesome due to the high order of coefficients matrix, so that a number of procedures have to be used in order to reduce the computational cost of minimization. Anyway, analyzing these methods is beyond the scope of this book. It is sufficient for the reader to know that this is a task of the software that he/she uses to apply the FEM, and all the information about the implemented minimization algorithms is usually described in the documentation of the software.

2.3 Use of FEM for the Analysis of Waves Propagation

Typically, the wave propagation phenomena are described by the Helmholtz's equation:

$$\nabla^2 \Phi + k^2 \Phi = g \quad (2.13)$$

where Φ is field variable and g is the source function. It is possible to demonstrate that the functional corresponding to Eq. (2.13) is equal to:

$$I(\Phi) = \frac{1}{2} \iint \left[|\nabla \Phi|^2 - k^2 \Phi^2 + 2\Phi g \right] dS. \quad (2.14)$$

We need to express both the field variable and the source function in terms of shape functions over a triangular element:

$$\begin{aligned} \Phi_e(x, y) &= \sum_{i=1}^3 \alpha_i \Phi_{ei} \\ g_e(x, y) &= \sum_{i=1}^3 \alpha_i g_{ei}. \end{aligned}$$

The functional in Eq. (2.14), calculated for the single element, becomes:

$$I(\Phi_e) = \frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 \Phi_{ei} \Phi_{ej} \iint \nabla \alpha_i \nabla \alpha_j dS -$$

$$\begin{aligned} & \frac{k^2}{2} \sum_{i=1}^3 \sum_{j=1}^3 \Phi_{ei} \Phi_{ej} \iint \alpha_i \alpha_j dS + \\ & \sum_{i=1}^3 \sum_{j=1}^3 \Phi_{ei} g_{ej} \iint \alpha_i \alpha_j dS. \end{aligned} \quad (2.15)$$

Let us define $C_{ij} = \iint \nabla \alpha_i \cdot \nabla \alpha_j dS$ and $T_{ij} = \iint \alpha_i \cdot \alpha_j dS$.

The Eq. (2.15) can be then rewritten in matrix form:

$$I(\Phi_e) = \frac{1}{2} \Phi_e^T [C_e] \Phi_e - \frac{k^2}{2} \Phi_e^T [T_e] \Phi_e + \Phi_e^T [T_e] G_e. \quad (2.16)$$

By assembling such functional for all the elements, one gets

$$I(\Phi) = \frac{1}{2} \Phi^T [C] \Phi - \frac{k^2}{2} \Phi^T [T] \Phi + \Phi^T [T] G. \quad (2.17)$$

Once again, in order to find the solution of the wave problem, the derivative of Eq. (2.17) has to be taken with respect to all the free nodes. By splitting the vector Φ into a free and a prescribed subsets Φ_f and Φ_p , also the matrices $[C]$ and $[T]$ are consequently subdivided according to the fact that the entries multiply only free components, only prescribed ones or both in Eq. (2.17). An important class of problems is represented by the cases where the source term is null. In such cases, Eq. (2.17) can be rewritten as:

$$I(\Phi) = \frac{1}{2} [\Phi_f^T \Phi_p^T] \begin{bmatrix} C_{ff} & C_{fp} \\ C_{pf} & C_{pp} \end{bmatrix} \begin{bmatrix} \Phi_f \\ \Phi_p \end{bmatrix} - \frac{k^2}{2} [\Phi_f^T \Phi_p^T] \begin{bmatrix} T_{ff} & T_{fp} \\ T_{pf} & T_{pp} \end{bmatrix} \begin{bmatrix} \Phi_f \\ \Phi_p \end{bmatrix}. \quad (2.18)$$

In order to minimize this functional, the derivatives with respect to the free nodes have to be set equal to 0. We obtain:

$$\nabla I(\Phi) = [C_{ff} C_{fp}] \begin{bmatrix} \Phi_f \\ \Phi_p \end{bmatrix} - k^2 [T_{ff} T_{fp}] \begin{bmatrix} \Phi_f \\ \Phi_p \end{bmatrix} = 0 \quad (2.19)$$

which is a system of linear equations. We can further specialize Eq. (2.19) by assuming that the prescribed values are all equal to 0. In this case, we obtain:

$$\nabla I(\Phi) = [[C_{ff}] - k^2 [T_{ff}]] \Phi_f = 0 \quad (2.20)$$

which is a standard eigenproblem [2, 10].

2.4 Developing the FEM Model for a Wave Propagation Problem

In order to study a wave propagation problem using FEM, the steps to be performed will be illustrated below [7, 17]. These steps reflect the procedure commonly followed by the commercial packages, such as described in the Appendix for the software COMSOL™.

First of all we need to define a coordinates system. More specifically, we need to choose how many dimensions have to be considered. Because the 3D geometry is usually a large computational problem, it would be better to avoid it if possible. One needs to exploit symmetries in order to create 2D or 2D axisymmetric geometries that involve a lower computational cost.

After that we need to define the relevant physics involved in the problem. In general, the software gives in hand a collection of specific modules for each physics, so in general, one needs just to select the proper module/modules.

At this point, the PDE and the number of spatial dimensions have been chosen. For acoustic pressure, the PDE is the Helmholtz's equation (1.13) in Chap. 1, that is obtained by considering a constant density value.

This equation governs the spatial dependency of p , which permits us to know p completely, since the temporal part is already known. The goal is then to solve Eq. (1.14), defined in Chap. 1, for the frequencies of interest.

For axisymmetric geometries, the axis of symmetry is $r = 0$. For the acoustic pressure in 2D axisymmetric geometries, the wave equation becomes:

$$\frac{\partial}{\partial r} \left(-\frac{r}{\rho} \frac{\partial p}{\partial r} \right) + r \frac{\partial}{\partial r} \left(-\frac{1}{\rho} \frac{\partial p}{\partial z} \right) - \left[\left(\frac{\omega}{c} \right)^2 - \left(\frac{m}{r} \right)^2 \right] \frac{rp}{\rho} = 0 \quad (2.21)$$

where m denotes the circumferential wave number. In this case, k_z is the out-of-plane wave number. In 2D axisymmetric geometries, the independent variables are the radial coordinate r and the axial coordinate z .

It is a very good approach to parameterize all the dimensions and link them together in order to easily change the geometry lately. The other way is to design the device using specialized computer-aided design (CAD) software and then import the geometry in the FEM software.

The various regions must match the materials they represent. The material properties represent all the constants that appear in the PDE. The type of material can be chosen among those already present in the database, or one can create his/her own materials, specifying the properties that have to be used during the analysis.

For acoustic pressure, the principal properties of the medium are density and speed of sound.¹

¹ If the problem needs to be coupled, others properties are to be entered. For example, if a coupled thermal problem is studied, the density and the speed of sound could be functions of temperature.

Initial conditions are used in conjunction with time studies and this condition adds initial values for the sound pressure p and the pressure time derivative dp/dt that can serve as an initial guess for a nonlinear solver.

Boundary conditions define the nature of the boundaries of the computational domain. Some define real physical obstacles like a sound hard wall or a moving interface. Others, called artificial boundary conditions, are used to truncate the domain. The artificial boundary conditions are, for example, used to simulate an open boundary where no sound is reflected. For acoustic pressure mode, it is possible to choose among the following boundary conditions [6]:

- **Neumann Condition**

The normal component of particle velocity disappears. This condition is equivalent to the normal acceleration equal to 0:

$$n \cdot \left(\frac{1}{\rho_0} (\nabla p) - q \right) = 0.$$

If the dipole source q is null, the normal derivative of the pressure is equal to 0:

$$\frac{dp}{dn} = 0 \quad (\text{normal velocity} = 0).$$

This condition is used to model rigid surfaces.

- **Dirichlet Condition**

This condition nullifies in the boundary the acoustic pressure value:

$$p = 0.$$

It is an appropriate approximation for a liquid–gas interface.

- **Pressure (Dirichlet Condition) $p = p_0$**

The pressure condition specifies in the boundary, the acoustic pressure amplitude (oscillating as $e^{i\omega t}$) in the frequency analysis. In the transient analysis, the time dependence of the pressure source has to be explicated.

- **Normal Acceleration (Neumann Condition)**

This condition sets the inward normal acceleration amplitude at the boundary:

$$n \cdot \left(\frac{1}{\rho_0} (\nabla p) \right) = a_n \tag{2.22}$$

where a_n represents an external source term.

Using this condition, it is possible to obtain also an acoustic source: a sound can be produced through the vibration of the boundary (e.g., a baffled piston or a desired simple source strength if a small boundary is selected).

This condition is used to couple acoustic domains to adjacent mechanical domains through a function that sets the acceleration on the boundary of the latter as the condition (see Sect. 2.5).

Ultrasonic Nondestructive Evaluation Systems

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