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COMPUTATIONAL MODELING OF TRANSIENT ACOUSTIC WAVEFIELDS - A STRUCTURED APPROACH BASED ON RECIPROCITY

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The reciprocity theorem for transient acoustic wavefields is taken as the point of departure for developing computational methods to model such wavefields. Mathematically, the theorem is representative of any 'weak' formulation of the wavefield problem. Physically, the theorem describes the 'interaction' between (a discretized version of) the actual wavefield and a suitably chosen 'computational state'. The choice of the computational state determines which type of computational method results from the analysis. It is shown that the finite-element method, the integral-equation method and the domain integration method can be viewed upon as particular cases of discretizing the reciprocity relation. The local field representations of the acoustic pressure and the particle velocity in terms of nodal- and face-element expansion functions, respectively, are worked out in some detail. The emphasis is on time-domain methods. The relationship with complex frequency-domain methods is indicated.

1. Introduction

The local, pointwise behavior in space-time of acoustic wavefields is governed by a hyperbolic system of first-order partial differential equations (equation of motion and deformation rate equation) that are representative for the acoustic wave phenomena on a local scale. When supplemented with the boundary conditions that join the wavefield values on either side of the interfaces where the constitutive parameters jump by finite amounts, and by requiring causality of the relationship between the wavefield and its generating sources, the problem has a unique solution. A number of properties of this solution, in particular its analyticity and reciprocity properties follow from this description. The computational handling of the wavefield problem, however, often starts from a 'weak' formulation, where the pointwise, or 'strong', satisfaction of the equality signs in the equations is replaced with requirements on the equality of certain integrated, or weighted, versions of the differential equations. Such weighted versions can be considered as special cases of the global reciprocity theorem that applies to two different admissible wavefield 'states' that are defined in one and the same domain in configuration space. Conceptually, a computational scheme to evaluate the wavefield is then taken to describe the interaction between (a discretized version of) the actual wavefield state and a suitably chosen 'computational state'. The latter is representative of the method at hand (for example, finite-element method and its related method of weighted residuals, integral-equation method, domain integration method). Thus, choosing the reciprocity theorem as the point of departure offers the road to a structured approach to constructing computational schemes for evaluating the wavefield. Besides, the standard source/receiver reciprocity properties (which are also consequences of the reciprocity theorem) can serve as a check on the consistency of the numerical results obtained.

The emphasis is on time-domain methods. The relationship with complex frequency-domain methods is indicated.

2. The acoustic wavefield

The acoustic wavefield under consideration is present in three-dimensional Euclidean space $\mathcal{R}^3$. The distribution of matter in it is assumed to be time invariant and the materials are assumed to be linear in their acoustic behavior. Position in the configuration is specified by the coordinates $\{x_1, x_2, x_3\}$ with respect to an orthogonal, Cartesian reference frame with the origin $\mathcal{O}$ and the three, mutually perpendicular base vectors $\{\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3\}$ of unit length each. In the indicated order, the base vectors form a right-handed system. The corresponding position vector is $\boldsymbol{x} = x_1\boldsymbol{i}_1 + x_2\boldsymbol{i}_2 + x_3\boldsymbol{i}_3$. The time coordinate is t. The subscript notation for vectors and tensors is used and the summation convention applies. Differentiation with respect to x_m is denoted by ∂_m; ∂_t is a reserved symbol for differentiation with respect to t.

The acoustic constitutive properties of the media in the configuration are characterized by their volume density of mass $\rho_{k,r} = \rho_{k,r}(\boldsymbol{x})$ and their compressibility $\kappa = \kappa(\boldsymbol{x})$. The tensorial volume density of mass has been included in the analysis rather than its scalar counterpart to accomodate the 'equivalent fluid approximation' for compressional acoustic waves in anisotropic elastic solids such as fluid/solid layered rock (De Hoop 1995a). The volume density of mass is taken to be a positive definite, symmetric tensor of rank two, the compressibility is taken to be a positive scalar. The action of the sources that generate the wavefield is characterized by the volume source density of (external) force $f_k = f_k(\boldsymbol{x}, t)$ (acoustic dipole type sources) and the volume source density of (external) volume injection rate $q = q(\boldsymbol{x}, t)$ (acoustic monopole type sources). In each subdomain of the configuration where the constitutive coefficients vary continuously with position, the wavefield quantities acoustic pressure $p = p(\boldsymbol{x}, t)$ and particle velocity $v_r = v_r(\boldsymbol{x}, t)$ then satisfy the hyperbolic system of partial differential equations (De Hoop 1995b)

$$\partial_k p + \rho_{k,r}\partial_t v_r = f_k, \tag{1}$$

$$\partial_r v_r + \kappa\partial_t p = q. \tag{2}$$

The existence of solutions of these wavefield equations is subject to the satisfaction of the compatibility relation

$$\epsilon_{j,m,k}\partial_m(\rho_{k,r}\partial_t v_r) = \epsilon_{j,m,k}\partial_m f_k, \tag{3}$$

where $\epsilon_{j,m,k}$ is the completely antisymmetric unit tensor of rank three (Levi-Civita tensor): $\epsilon_{j,m,k} = +1$ if $\{j, m, k\}$ is an even permutation of $\{1, 2, 3\}$, $\epsilon_{j,m,k} = -1$ if $\{j, m, k\}$ is an odd permutation of $\{1, 2, 3\}$, $\epsilon_{j,m,k} = 0$ in all other cases. Across interfaces where $\rho_{k,r}$ and/or κ jump by finite amounts the wavefield quantities are no longer continuously differentiable and the boundary conditions

$$p = \text{continuous}, \tag{4}$$

$$\nu_r v_r = \text{continuous}, \tag{5}$$

should be satisfied. Here, ν_r is the unit vector along the normal to the interface. If the configuration extends to infinity, it is assumed that in the domain $\mathcal{D}^{\mathrm{b}}$ (the 'embedding') outside some bounded closed surface $\partial\mathcal{D}^{\mathrm{b}}$ the medium is such that the pertaining tensor Green's functions are analytically known. As a consequence, analytic source-type integral representations for the wavefield quantities in $\mathcal{D}^{\mathrm{b}}$ exist. The latter play a role in the *contrast source* or *scattering* formulation of the wavefield problem.

In the analysis, the *time convolution* operator is needed. For any two space-time functions $F(\boldsymbol{x}, t)$ and $Q(\boldsymbol{x}, t)$ this operator is defined through

$$\mathrm{C}_t(F, Q; \boldsymbol{x}, t) = \int_{t' \in \mathcal{R}} F(\boldsymbol{x}, t')Q(\boldsymbol{x}, t - t')\mathrm{d}t' \quad \text{for } t \in \mathcal{R}. \tag{6}$$

It has the properties

$$\mathrm{C}_t(F, Q; \boldsymbol{x}, t) = \mathrm{C}_t(Q, F; \boldsymbol{x}, t), \tag{7}$$

$$\partial_t\mathrm{C}_t(F, Q; \boldsymbol{x}, t) = \mathrm{C}_t(\partial_t F, Q; \boldsymbol{x}, t) = \mathrm{C}_t(F, \partial_t Q; \boldsymbol{x}, t). \tag{8}$$

For *causal* space-time functions $F(\boldsymbol{x},t)$ and $Q(\boldsymbol{x},t)$, having the semi-infinite interval $\{t \in \mathcal{R}; t > 0\}$ as their supports, $\mathrm{C}_t(F,Q;\boldsymbol{x},t)$ is causal as well, with the same support.

The relation between the time-domain quantities and their complex frequency-domain counterparts is given by the time Laplace transformation, which for any space-time function $F(\boldsymbol{x},t)$ is

$$\hat{F}(\boldsymbol{x},s) = \int_{t\in\mathcal{R}} \exp(-st)F(\boldsymbol{x},t)\mathrm{d}t \quad \text{for } \mathrm{Re}(s) = s_0, \tag{9}$$

where s_0 is some real value of $s \in \mathcal{C}$ for which the integral on the right-hand side is convergent. For *causal*, bounded, space-time functions $F(\boldsymbol{x},t)$ having the semi-infinite interval $\{t \in \mathcal{R}; t > 0\}$ as their support, $\hat{F}(\boldsymbol{x},s)$ is analytic in the right half $\{s \in \mathcal{C}; \mathrm{Re}(s) > 0\}$ of the complex s-plane. The Laplace transform $\widehat{\mathrm{C}_t}(F,Q;\boldsymbol{x},s)$ of $\mathrm{C}_t(F,Q;\boldsymbol{x},t)$ is from Equations (6) and (9) found as

$$\widehat{\mathrm{C}_t}(F,Q;\boldsymbol{x},s) = \hat{F}(\boldsymbol{x},s)\hat{Q}(\boldsymbol{x},s). \tag{10}$$

Further, the Laplace transform $\widehat{\partial_t F}(\boldsymbol{x},s)$ of $\partial_t F(\boldsymbol{x},t)$ is from Equation (9) and a subsequent integration by parts found as

$$\widehat{\partial_t F}(\boldsymbol{x},s) = s\hat{F}(\boldsymbol{x},s). \tag{11}$$

With the aid of this latter rule, the complex frequency-domain wavefield equations are from Equations (1) - (2), (9) and (11) obtained as

$$\partial_k \hat{p} + s\rho_{k,r}\hat{v}_r = \hat{f}_k, \tag{12}$$

$$\partial_r \hat{v}_r + s\kappa\hat{v}_r = \hat{q}, \tag{13}$$

while the complex frequency-domain compatibility relation is from Equations (3), (9) and (11) obtained as

$$s\epsilon_{j,m,k}\partial_m(\rho_{k,r}\hat{v}_r) = \epsilon_{j,m,k}\partial_m \hat{f}_k. \tag{14}$$

The boundary conditions across interfaces in jumps of the constitutive coefficients are from Equations (4) - (5), (9) and (11) obtained as

$$\hat{p} = \text{continuous}, \tag{15}$$

$$\nu_r\hat{v}_r = \text{continuous}. \tag{16}$$

3. The reciprocity theorem

In the reciprocity theorem (that is named after Lord Rayleigh) a certain *interaction quantity* is considered that is representative for the interaction between two admissible solutions ('states') of the field equations, where the latter are defined in one and the same (proper or improper) subdomain $\mathcal{D}$ of $\mathcal{R}^3$. The domain $\mathcal{D}$ is assumed to be the union of a finite number of subdomains in each of which the wavefield quantities of the two states are continuously differentiable. Furthermore, each of the two states applies to its own medium and has its own volume source distributions. The two states will be indicated by the superscripts A and Z, respectively (Figure 1). The relevant local interaction quantity is $\partial_m[\mathrm{C}_t(p^A, v_m^Z) - \mathrm{C}_t(p^Z, v_m^A)]$ (De Hoop 1988, 1995c). Using the standard rules for the spatial differentiation and employing the wavefield equations of the type (1)-(2) for the two states, it is found that

$$\begin{aligned}&\partial_m[\mathrm{C}_t(p^A, v_m^Z) - \mathrm{C}_t(p^Z, v_m^A)]\\&= (\rho_{r,k}^Z - \rho_{k,r}^A)\mathrm{C}_t(v_r^A, v_k^Z) - (\kappa^Z - \kappa^A)\partial_t\mathrm{C}_t(p^A, p^Z)\\&\quad+\mathrm{C}_t(f_k^A, v_k^Z) - \mathrm{C}_t(q^A, p^Z) - \mathrm{C}_t(f_r^Z, v_r^A) + \mathrm{C}_t(q^Z, p^A).\end{aligned} \tag{17}$$

Equation (17) is the *local form of the acoustic reciprocity theorem of the time-convolution type.* The first two terms on the right-hand side are representative of the differences (contrasts) in the acoustic properties of the media in the two states; these terms vanish at those positions where $\rho_{r,k}^Z(\boldsymbol{x}) = \rho_{k,r}^A(\boldsymbol{x})$ and $\kappa^Z(\boldsymbol{x}) = \kappa^A(\boldsymbol{x})$. At points where these latter conditions hold, the media are denoted as each other's *adjoints.* The last four terms on the right-hand side are representative for the action of the volume sources in the two states; these terms vanish at those positions where the wavefield is sourcefree.

To arrive at the global form of the reciprocity theorem for some bounded domain $\mathcal{D}$, it is assumed that $\mathcal{D}$ is the union of a finite number of subdomains in each of which the terms in Equation (17) are continuous. Upon integrating Equation (17) over each of these subdomains, applying Gauss' integral theorem to the resulting left-hand sides, and adding the results, it follows that

$$\begin{aligned}&\int_{\partial\mathcal{D}} \nu_m[\mathrm{C}_t(p^A, v_m^Z) - \mathrm{C}_t(p^Z, v_m^A)]\mathrm{d}A(\boldsymbol{x})\\&= \int_{\mathcal{D}}[(\rho_{r,k}^Z - \rho_{k,r}^A)\mathrm{C}_t(v_r^A, v_k^Z) - (\kappa^Z - \kappa^A)\partial_t\mathrm{C}_t(p^A, p^Z)]\mathrm{d}V(\boldsymbol{x})\\&\quad+\int_{\mathcal{D}}[\mathrm{C}_t(f_k^A, v_k^Z) - \mathrm{C}_t(q^A, p^Z) - \mathrm{C}_t(f_r^Z, v_r^A) + \mathrm{C}_t(q^Z, p^A)]\mathrm{d}V(\boldsymbol{x}).\end{aligned} \tag{18}$$

Equation (18) is the *global form, for the domain $\mathcal{D}$, of the reciprocity theorem of the time-convolution type.* Note that in the process of adding the contributions from the subdomains of $\mathcal{D}$, the contributions from common interfaces have canceled in view of the boundary conditions (4) - (5). In view of this, in the left-hand side only a contribution from the outer boundary $\partial\mathcal{D}$ of $\mathcal{D}$ remains.

The complex frequency-domain versions of the local and the global reciprocity theorems follow from their time-domain counterparts by taking the time Laplace transform.

Applying the standard rules given in Section 2, the complex frequency-domain version of the local reciprocity theorem follows from Equation (17) as

$$\begin{aligned}&\partial_m(\hat{p}^A\hat{v}_m^Z - \hat{p}^Z\hat{v}_m^A)\\ &= s(\rho_{r,k}^Z - \rho_{k,r}^A)\hat{v}_r^A\hat{v}_k^Z - s(\kappa^Z - \kappa^A)\hat{p}^A\hat{p}^Z\\ &\quad + \hat{f}_k^A\hat{v}_k^Z - \hat{q}^A\hat{p}^Z - \hat{f}_r^Z\hat{v}_r^A + \hat{q}^Z\hat{p}^A.\end{aligned} \tag{19}$$

and the complex frequency-domain version of the global reciprocity theorem from Equation (18) as

$$\begin{aligned}&\int_{\partial\mathcal{D}} \nu_m(\hat{p}^A\hat{v}_m^Z - \hat{p}^Z\hat{v}_m^A)\mathrm{d}A(\boldsymbol{x})\\ &= \int_{\mathcal{D}}[s(\rho_{r,k}^Z - \rho_{k,r}^A)\hat{v}_r^A\hat{v}_k^Z - s(\kappa^Z - \kappa^A)\hat{p}^A\hat{p}^Z]\mathrm{d}V(\boldsymbol{x})\\ &\quad + \int_{\mathcal{D}}(\hat{f}_k^A\hat{v}_k^Z - \hat{q}^A\hat{p}^Z - \hat{f}_r^Z\hat{v}_r^A + \hat{q}^Z\hat{p}^A)\mathrm{d}V(\boldsymbol{x}).\end{aligned} \tag{20}$$

The limiting case of an unbounded domain

In quite a number of cases, the global reciprocity theorems will be applied to an unbounded domain. To handle such cases, the embedding provisions of Section 2 are made and the theorem is first applied to the sphere $\mathcal{S}(\mathcal{O},\Delta)$ with center at the origin $\mathcal{O}$ of the chosen reference frame and radius Δ, after which the limit $\Delta \to \infty$ is taken. From the source-type field integral representations pertaining to the embedding (in particular, from the one applying to a homogeneous, isotropic embedding) it then follows that the contribution from $\mathcal{S}(\mathcal{O},\Delta)$ vanishes in the limit $\Delta \to \infty$.

In the above procedure, the acoustic wavefield equations pertaining to the two states have been taken as the point of departure and the reciprocity theorems have been derived by operating on the equations in the manner indicated. In the realm of the use of the reciprocity theorems as the basis of a structured approach to the computation of the fields, it is important to notice that, reversely, a necessary and sufficient condition for the global reciprocity theorem for arbitrary acoustic states Z satisfying equations of the type (1) - (2) and boundary conditions of the type (4) - (5) to hold, is that the field in State A satisfies equations of the type (1) - (2) and boundary conditions of the type (4) - (5) as well.

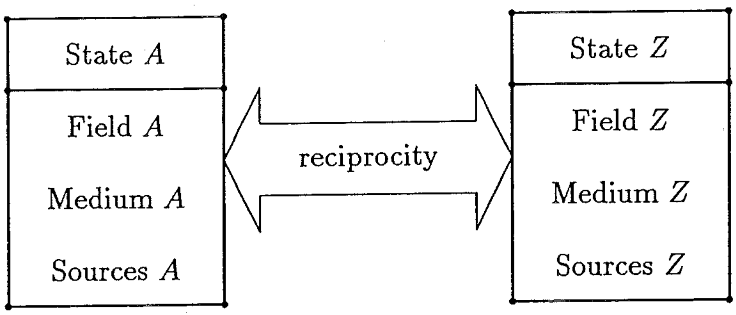

Figure 1. The two admissible states in the reciprocity theorem.

4. Embedding procedure and contrast source formulations

On many occasions the computation of an acoustic wavefield in an entire configuration is beyond the capabilities because of the storage capacity and the computation times involved. In that case it is standard practice to select a *target region* of bounded support in which a detailed computation is to be carried out, while the medium in the remaining part of the configuration (the *embedding*) is taken so simple that the field in it can be determined with the aid of analytical methods. Examples of such embeddings in $\mathcal{R}^3$ as the configuration space are: the homogeneous, isotropic embedding, and the embedding consisting of a finite number of parallel, homogeneous layers. In these cases, combined time Laplace and spatial Fourier transform techniques provide the analytical tools to determine the field or, in fact, construct the relevant Green's tensors. Once the embedding has been chosen, the problem of computing the wavefield in the target region can advantageously be formulated as a *contrast-source* or *scattering* problem (De Hoop, 1995d).

To this end, first the *incident wavefield* $\{p^{\mathrm{i}}, v_r^{\mathrm{i}}\}$ is introduced as the wavefield that would be generated by the sources as if they were present in the embedding. Let $\rho_{k,r}^{\mathrm{b}} = \rho_{k,r}^{\mathrm{b}}(\boldsymbol{x})$ and $\kappa^{\mathrm{b}} = \kappa^{\mathrm{b}}(\boldsymbol{x})$ be the constitutive parameters of the embedding occupying the domain $\mathcal{D}^{\mathrm{b}}$. Then, the incident wavefield satisfies the basic wavefield equations

$$\partial_k p^{\mathrm{i}} + \rho_{k,r}^{\mathrm{b}} \partial_t v_r^{\mathrm{i}} = f_k, \tag{21}$$

$$\partial_r v_r^{\mathrm{i}} + \kappa^{\mathrm{b}} \partial_t p^{\mathrm{i}} = q. \tag{22}$$

Next, the *scattered wavefield* $\{p^{\mathrm{s}}, v_r^{\mathrm{s}}\}$ is defined as the difference between the total wavefield $\{p, v_r\}$ and the incident wavefield $\{p^{\mathrm{i}}, v_r^{\mathrm{i}}\}$. Hence, $\{p, v_r\} = \{p^{\mathrm{i}}+p^{\mathrm{s}}, v_r^{\mathrm{i}}+v_r^{\mathrm{s}}\}$. The wavefield equations for the scattered wavefield can alternatively be written as

$$\partial_k p^{\rm s} + \rho_{k,r}\partial_t v_r^{\rm s} = -(\rho_{k,r} - \rho_{k,r}^{\rm b})\partial_t v_r^{\rm i}, \tag{23}$$
$$\partial_r v_r^{\rm s} + \kappa\partial_t p^{\rm s} = -(\kappa - \kappa^{\rm b})\partial_t p^{\rm i}, \tag{24}$$

or as

$$\partial_k p^{\rm s} + \rho_{k,r}^{\rm b}\partial_t v_r^{\rm s} = -(\rho_{k,r} - \rho_{k,r}^{\rm b})\partial_t v_r, \tag{25}$$
$$\partial_r v_r^{\rm s} + \kappa^{\rm b}\partial_t p^{\rm s} = -(\kappa - \kappa^{\rm b})\partial_t p, \tag{26}$$

In both systems, the right-hand sides only differ from zero in the domain where the constitutive properties of the medium differ from those of the embedding. Further, in none of them the activating source distributions occur. This has the advantage of a smoother behavior of the right-hand sides of the differential equations, a behavior which is due to the fact that the (incident) wavefield varies more smoothly in space than its generating source distributions (Hohmann 1989). Equations (23) - (24) are typically the point of departure for finite-difference or finite-element computations; Equations (25) - (26) are typically the point of departure for integral-equation computations and for the construction of 'absorbing boundary conditions' or 'Dirichlet-to-Neumann maps'.

The source-type integral representations for the incident and the scattered wavefields are of the type

$$p^{\rm i,s}(\boldsymbol{x},t) = \int_{\mathcal{D}^{\rm i,s}} \{\mathrm{C}_t[G^{p,q}(\boldsymbol{x},\boldsymbol{x}',\cdot), q^{\rm i,s}(\boldsymbol{x}',\cdot)] + \mathrm{C}_t[G_k^{p,f}(\boldsymbol{x},\boldsymbol{x}',\cdot), f_k^{\rm i,s}(\boldsymbol{x}',\cdot)]\}\mathrm{d}V(\boldsymbol{x}'), \tag{27}$$
$$v_r^{\rm i,s}(\boldsymbol{x},t) = \int_{\mathcal{D}^{\rm i,s}} \{\mathrm{C}_t[G_r^{v,q}(\boldsymbol{x},\boldsymbol{x}',\cdot), q^{\rm i,s}(\boldsymbol{x}',\cdot)] + \mathrm{C}_t[G_{r,k}^{v,f}(\boldsymbol{x},\boldsymbol{x}',\cdot), f_k^{\rm i,s}(\boldsymbol{x}',\cdot)]\}\mathrm{d}V(\boldsymbol{x}'), \tag{28}$$

where $\mathcal{D}^{\rm i}$ is the support of the volume source densities

$$f_k^{\rm i} = f_k, \tag{29}$$
$$q^{\rm i} = q, \tag{30}$$

generating the incident wavefield, $\mathcal{D}^{\rm s}$ is the support of the contrast volume source densities

$$f_k^{\rm s} = -(\rho_{k,r} - \rho_{k,r}^{\rm b})\partial_t v_r, \tag{31}$$
$$q^{\rm s} = -(\kappa - \kappa^{\rm b})\partial_t p, \tag{32}$$

generating the scattered wavefield, and $G^{p,q}, G_k^{p,f}, G_r^{v,q}, G_{r,k}^{v,f}$ are the acoustic-pressure/ injection-source, acoustic-pressure/force-source, particle-velocity/injection-source, particle-velocity/force-source Green's tensors of the embedding.

The complex frequency-domain versions of Equations (21) - (32) are found from their time-domain counterparts by replacing the operator ∂_t by the multiplying factor s and replacing the time convolutions by the product of their operands.

5. Computational procedures based on reciprocity

In the structured approach to the development of computational procedures based on reciprocity, the first step consists of selecting, in the global reciprocity theorems derived in Section 3, a finite number of linearly independent computational states for the State Z. The relevant states will be indicated by the superscript C and their number is taken to be N^C. Next, State A is taken to be an approximation to the scattered field as introduced in Section 4, in the form of an expansion into a sequence of appropriate, linearly independent, known, expansion functions and provided with unknown expansion coefficients. The relevant state will be indicated by the superscript s and its field representation will contain N^{s} terms. Based on the knowledge (see the end of Section 3) that for any number of arbitrary computational states and with an appropriate expansion containing an infinite number of terms for the scattered state, the application of the reciprocity theorem would lead to the unique, exact solution of the field problem, it is now assumed that the procedure with a finite number of computational states and a finite number of terms in the expansion of the scattered state leads to an 'approximate solution' to the field problem. A quantification of the resulting 'error' can only be decided upon after having introduced an appropriate 'error criterion'. The latter is beyond the scope of the present analysis, which is mainly focused on the construction of both the computational states and 'appropriate' expansion functions. Right from the beginning it is clear that for $N^C < N^{\mathrm{s}}$ the system of linear, algebraic equations in the expansion coefficients is underdetermined and hence cannot be solved, while for $N^C = N^{\mathrm{s}}$ the system of linear, algebraic equations in the expansion coefficients has in principle a unique solution, whereas for $N^C > N^{\mathrm{s}}$ the system of linear, algebraic equations in the expansion coefficients is overdetermined and is, hence, amenable to a minimum norm solution in its residual.

The computations are generally carried out on a geometrically discretized version of the configuration. To this end, first the target region or domain of computation $\mathcal{D}$ is selected and discretized (Figure 2). The boundary surface $\partial\mathcal{D}$ of this domain is taken to be located in the embedding $\mathcal{D}^{\mathrm{b}}$. Its geometrical shape is taken such that it can be handled by a *mesh generator*. Typical cases are the discretization into a union of 3-rectangles or 3-simplices (tetrahedra), all of which have vertices, edges and faces in common (Naber 1980). The maximum diameter of the elements of the discretized geometry is denoted as its *mesh size*. The mesh size depends on the shape of $\partial\mathcal{D}$, as well as on the spatial variations of the constitutive coefficients and the temporal and spatial variations of the volume source densities and the field values in $\mathcal{D}$.

The mesh size is first adapted to the spatial variations of the known quantities (constitutive coefficients and volume source densities in forward problems, volume source densities and measured field values in inverse problems) and later iteratively adapted to the quantities to be computed (field values in forward problems, constitutive coefficients in inverse problems). Coupled to the mesh are, next, the spatial and temporal representations of the discretized known quantities. Finally, the discretized versions of the computational states and the unknown quantities are selected.

To illustrate the procedure, the forward wavefield problem will be discussed in more detail below. More details about handling acoustic inverse source and inverse wave scattering problems can be found in De Hoop (1988, 1995e).

It is implied that the incident field has been determined already by an appropriate integration procedure applied to the pertaining source-type integral representations containing the analytically known Green's tensors of the embedding (see Section 4).

In the forward wavefield computation problem, the constitutive coefficients and the volume source distributions are given, and the field values are to be computed. As far as the medium properties are concerned, the analysis will be concentrated on the case of strongly heterogeneous media where the constitutive coefficients may, in principle, jump from each subdomain of the discretized geometry to any adjacent subdomain. The mesh size is assumed to be chosen so small that *piecewise linear expansions* suffice to locally represent the field values, the constitutive coefficents and the volume source densities. A consistent theory can then be developed for a *simplicial mesh* consisting of 3-simplices (tetrahedra) all of which have vertices, edges and faces in common (Figure 3).

Consider one of the tetrahedra, Σ say, of the mesh and let $\{x_m(0), x_m(1), x_m(2), x_m(3)\}$ be the position vectors of its vertices. The ordering in the sequence defines the *orientation* of the tetrahedron. Let, further, $\{A_m(0), A_m(1), A_m(2), A_m(3)\}$ denote the outwardly oriented vectorial areas of the faces of Σ, where the ordinal number of a face is taken to be the ordinal number of the vertex opposite to it. The position vector $\boldsymbol{x}$ in Σ can then in a symmetrical fashion be expressed in terms of the *barycentric coordinates* $\{\lambda(0,\boldsymbol{x}), \lambda(1,\boldsymbol{x}), \lambda(2,\boldsymbol{x}), \lambda(3,\boldsymbol{x})\}$ through

$$x_m = \sum_{I=0}^{3} \lambda(I,\boldsymbol{x}) x_m(I). \tag{33}$$

Inversely, the barycentric coordinates can be expressed in terms of the position vector via the relation

$$\lambda(I,\boldsymbol{x}) = 1/4 - (1/3V)(x_m - b_m)A_m(I) \quad \text{for } I = 0,1,2,3, \tag{34}$$

where V is the volume of Σ and

$$b_m = \frac{1}{4}\sum_{I=0}^{3} x_m(I) \tag{35}$$

is the position vector of its *barycenter*. The barycentric coordinates have the property

$$\lambda(I,\boldsymbol{x}(J)) = \delta(I,J) \quad \text{for } I = 0,1,2,3;\ J = 0,1,2,3, \tag{36}$$

where $\delta(I,J)$ is the Kronecker symbol: $\delta(I,J)=1$ for $I=J$ and $\delta(I,J)=0$ for $I\neq J$.

As Equations (33) and (36) show, the barycentric coordinates perform a linear interpolation, in the interior of Σ, between the function value one at one of the vertices and the function value zero at the remaining vertices. Consequently, they can be used as the (linear) interpolation functions for any of the quantities occurring in the field computation. As an example of a scalar quantity, the acoustic pressure is considered. This quantity admits the local representation

$$p(\boldsymbol{x},t)=\sum_{I=0}^{3} A^{p}(I,t)\lambda(I,\boldsymbol{x}) \quad \text{for } \boldsymbol{x}\in\Sigma, \tag{37}$$

where

$$A^{p}(I,t)=p(\boldsymbol{x}(I),t) \quad \text{for } I=0,1,2,3. \tag{38}$$

As an example of a vectorial quantity, the particle velocity is considered. This quantity admits the local representation

$$v_r(\boldsymbol{x},t)=\sum_{I=0}^{3} A^{v}_{r}(I,t)\lambda(I,\boldsymbol{x}) \quad \text{for } \boldsymbol{x}\in\Sigma, \tag{39}$$

where

$$A^{v}_{r}(I,t)=v_r(\boldsymbol{x}(I),t) \quad \text{for } I=0,1,2,3. \tag{40}$$

From the *local* representations of the type (37) - (39) the *global* representations for the domain of computation are constructed. In this process, the values of the constitutive coefficients and the volume source densities in the interior of the tetrahedron Σ, and hence their limiting values upon approaching (via the interior) the vertices of Σ, have no relation to the values of these quantities in any of the neighbors of Σ. As a consequence, each nodal point of the mesh is, for these quantities, initially considered as a *multiple node*, with multiplicity equal to the number of vertices that meet at that point. Subsequently, the multiple nodes are combined to *simple nodes* in all those subdomains of the domain of computation where the quantities are known to be continuous. For the acoustic pressure and the particle velocity the situation shows, however, additional features. These quantities vary continously in space as long as the constitutive coefficients do so (even if the volume source densities vary only piecewise continuously in space), but across a jump discontinuity in constitutive properties of the medium, the acoustic pressure and the normal component of the particle velocity are to be continuous, while the tangential component of the particle velocity should remain free to jump. A representation that meets these requirements is furnished by using for the acoustic pressure the *nodal-element representation* as given by Equation (37) and using for the particle velocity the *face-element representation*. In this representation, $A^{v}_{r}(I,t)=v_r(\boldsymbol{x}(I),t)$ is expressed in terms of its projections along the normals to the faces that meet at the vertex $\boldsymbol{x}(I)$. Rather than with these projections we work with the numbers

$$\alpha^v(I,J,t) = v_r(\boldsymbol{x}(I),t)A_r(J) \quad \text{for } I=0,1,2,3;\ J=0,1,2,3, \tag{41}$$

with $\alpha^v(I,I,t)=0$. In view of the fact that at the vertex $\boldsymbol{x}(I)$ the three vectorial edges $\{x_r(J)-x_r(I); J\neq I\}$ and the three vectorial faces $\{A_r(K); K\neq I\}$ form an (oblique) system of reciprocal base vectors in $\mathcal{R}^3$, the property

$$[x_m(J)-x_m(I)]A_m(K) = -3V[\delta(J,K)-\delta(I,K)] \quad \text{for } I=0,1,2,3;\ J=0,1,2,3;\ K=0,1,2,3, \tag{42}$$

holds. From Equations (39) - (42) it follows that

$$v_r(\boldsymbol{x}(I),t) = -\frac{1}{3V}\sum_{J=0}^{3}\alpha^v(I,J,t)[x_r(J)-x_r(I)] \quad \text{for } I=0,1,2,3. \tag{43}$$

Since $\alpha^v(I,I,t)=0$, we indeed have, through Equation (41), at each vertex three numbers that, through Equation (43), represent the expanded particle velocity. By enforcing the numbers along the normal to a particular face to be the same for the two tetrahedra that have this face in common, the continuity of the normal component of v_r across faces is guaranteed, while the tangential component of v_r across faces is left free to jump.

The piecewise linear expansions discussed above are used in the context of the different computational methods in existence. These will be briefly indicated below.

Finite-element method

The finite-element method is characterized by taking $\rho^C_{r,k}=0$ and $\kappa^C=0$ and choosing either

$$p^C \in \{\text{acoustic-pressure expansion functions}\}, \tag{44}$$
$$v^C_k = 0, \tag{45}$$
$$f^C_r = \partial_r p^C, \tag{46}$$
$$q^C = 0, \tag{47}$$

or

$$p^C = 0, \tag{48}$$
$$v^C_k \in \{\text{particle-velocity expansion functions}\}, \tag{49}$$
$$f^C_r = 0, \tag{50}$$
$$q^C = \partial_k v^C_k. \tag{51}$$

For this method, the choice of the acoustic pressure and the particle velocity typifies the computational state.

Integral-equation method

The integral-equation method is characterized by taking for the constitutive coefficients the values of the embedding, i.e. $\rho^C_{r,k} = \rho^{\mathrm{b}}_{r,k}$ and $\kappa^C = \kappa^{\mathrm{b}}$ and choosing either

$$
\begin{aligned}
f_r^C &\in \{\text{volume source of force expansion functions}\}, && (52)\\
q^C &= 0, && (53)\\
p^C(\boldsymbol{x},t) &= \int_{\mathcal{D}^f} \{\mathrm{C}_t[G_r^{p,f}(\boldsymbol{x},\boldsymbol{x}',\cdot), f_r^C(\boldsymbol{x}',\cdot)]\mathrm{d}V(\boldsymbol{x}'), && (54)\\
v_k^C(\boldsymbol{x},t) &= \int_{\mathcal{D}^f} \{\mathrm{C}_t[G_{k,r}^{v,f}(\boldsymbol{x},\boldsymbol{x}',\cdot), f_r^C(\boldsymbol{x}',\cdot)]\mathrm{d}V(\boldsymbol{x}'), && (55)
\end{aligned}
$$

where $\mathcal{D}^f$ is the support of f_r^C, or

$$
\begin{aligned}
f_r^C &= 0, && (56)\\
q^C &\in \{\text{volume source of injection rate expansion functions}\}, && (57)\\
p^C(\boldsymbol{x},t) &= \int_{\mathcal{D}^q} \{\mathrm{C}_t[G^{p,q}(\boldsymbol{x},\boldsymbol{x}',\cdot), q^C(\boldsymbol{x}',\cdot)]\mathrm{d}V(\boldsymbol{x}'), && (58)\\
v_k^C(\boldsymbol{x},t) &= \int_{\mathcal{D}^q} \{\mathrm{C}_t[G_k^{v,q}(\boldsymbol{x},\boldsymbol{x}',\cdot), q^C(\boldsymbol{x}',\cdot)]\mathrm{d}V(\boldsymbol{x}'), && (59)
\end{aligned}
$$

where $\mathcal{D}^q$ is the support of q^C. For this method, the choice of the volume source distributions, located in the embedding, typifies the computational state.

Domain integration method

The domain integration method is characterized by taking $\rho^C_{r,k} = 0$ and $\kappa^C = 0$ and choosing either

$$
\begin{aligned}
p^C &= \text{global constant with support } \mathcal{D}, && (60)\\
v_k^C &= 0, && (61)\\
f_r^C &= 0, && (62)\\
q^C &= 0, && (63)\\
& && (64)
\end{aligned}
$$

or

$$
\begin{aligned}
p^C &= 0, && (65)\\
v_k^C &= \text{global constant with support } \mathcal{D}, && (66)
\end{aligned}
$$

$$f_r^C = 0, \tag{67}$$
$$q^C = 0. \tag{68}$$
(69)

The value of the constant drops out from the final equations and the latter are equivalent to replacing the field equations by their integrated counterparts over the elementary subdomains of the domain of computation, applying Gauss' integral theorem, and adding the relevant results.

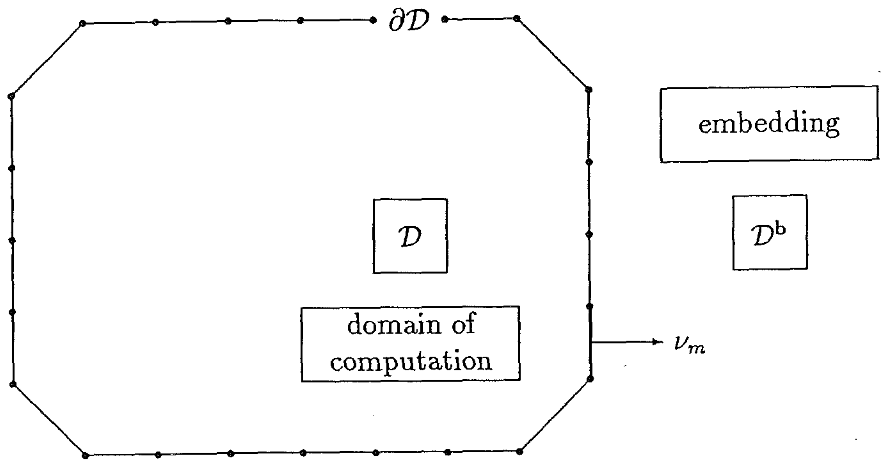

Figure 2. Discretized domain of computation $\mathcal{D}$ with boundary surface $\partial\mathcal{D}$ and embedding $\mathcal{D}^b$.

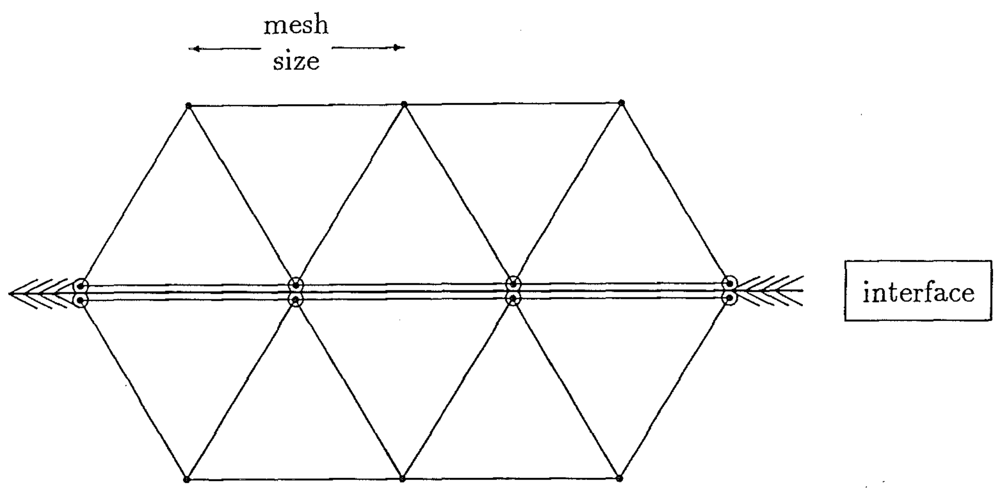

Figure 3. Interface ⋘ and simplicial mesh with multiple nodes ⊙ and simple nodes • .

6. Conclusion

A structured approach, with reciprocity as the basic principle, has been developed to construct schemes for the computation of acoustic wavefields. It is shown that the known algorithms concerning the finite-element, integral-equation, and domain integration technique all can be viewed upon as particular choices for the 'computational state' with which the 'interaction' of (the approximating expansion of) the actual field to be computed is set equal to zero. It is believed that the approach can also lead to additional types of algorithms.

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