Elastic Waves and Ultrasonic Nondestructive Evaluation
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RECIPROCITY, DISCRETIZATION, AND THE NUMERICAL SOLUTION OF ELASTODYNAMIC PROPAGATION AND SCATTERING PROBLEMS

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The larger part of wave propagation and scattering problems in elastodynamics has to be modeled with the aid of numerical methods. Many of these methods can be envisaged as being discretized versions of appropriate 'weak' formulations of the pertinent operator (differential or integral) equations. For the relevant problems as formulated in the time Laplace-transform domain it is shown that the Betti-Rayleigh reciprocity theorem encompasses all known weak formulations, while its discretization leads to the discretized form of the corresponding operator equations. The role of properly selected error criteria in the discretization procedures is emphasized.

1. INTRODUCTION

Except for the canonical problems whose solution can be expressed in terms of analytic functions of a not too complicated nature (examples of which can be found in Pao and Mow [**1**]) and for analytic approximation techniques (usually of an asymptotic nature), both in the long and the short wavelength regimes, that can be applied to a wider variety of cases, (see, for example, Achenbach, Gautesen and McMaken [**2**]) wave propagation and scattering problems in elastodynamics have to be addressed with the aid of numerical methods. Many of these methods can be envisaged as being discretized versions of appropriate 'weak' formulations of the pertinent operator (differential or integral) equations. Specifically, the finite-element method, based on the method of weighted residuals (see, for example, Zienkiewicz and Taylor [**3**]), applied to the elastodynamic partial differential equations, and the collocation method (method of point matching) applied to the source type elastodynamic integral relations (see, for example, Herman [**4**]) can be grouped in this category. The present paper is an attempt to systematize the different approaches and to bring, to a certain extent, consistency and coherence in the procedures.

To this end, the time Laplace-transform domain (s-domain) elastodynamic Betti-Rayleigh reciprocity theorem for time-invariant configurations is taken as point of departure. By taking the transform parameter s to be positive and real, as is done in the Cagniard method for calculating impulsive waves in stratified media (see, for example, Van der Hijden [**5**]]), or complex in the right half $\mathrm{Re}(s) > 0$ of the complex s-plane, the causality of the wave motion is ensured by requiring the time Laplace-transform domain wave field quantities to be bounded functions of position in space, especially at large distances from the sources (of bounded extent) that generate the wave field. Also, arbitrarily inhomogeneous and anisotropic materials with arbitrary relaxation behavior can in this way be incorporated in the analysis in an easy manner. From the s-domain results, the time-domain counterparts follow upon using some standard rules of the one-sided Laplace transformation, while the results for the limiting case of sinusoidally in time varying field quantities follow upon replacing s by $j\omega$, where j is the imaginary unit and ω the angular frequency of the oscillations, on the condition that imaginary values of s are approached via the right half of the complex s-plane.

Taking one of the two states in the reciprocity theorem to be the elastodynamic state to be actually computed and the other to be an 'auxiliary' or a 'computational' one, it is shown that the reciprocity theorem encompasses all known 'weak' formulations of the elastodynamic differential equations and source-type integral relations. For this reason, the Betti-Rayleigh reciprocity relation is considered to best serve as the point of departure for the computational modeling of elastodynamic wave fields. (Note that this theorem is global rather than local in nature.)

Turning to numerics, first a geometical discretization procedure is applied, with the

tetrahedron (simplex in three-dimensional space) as the basic building block. The mesh size of the discretization (maximum diameter of the tetrahedra) should be consistent with both the geometry of the configuration and the (inhomogeneous) distribution of matter in it, in the sense that it guarantees that the discretized configuration and the actual one differ relatively not more than a given fractional number according to some agreed-upon relative error criterion (for example, the relative root-mean-square error). Subsequently, the wave field to be computed is expanded in terms of a base in an appropriately chosen linear function space, and a weighting procedure with an appropriately chosen computational state is carried out. This procedure leads to a system of linear algebraic equations in the expansion coefficients. To solve this system of equations, again, an error criterion is needed to define what the 'best approximation' to the solution is (cf. Van den Berg [**6**]). In this manner, several versions of the finite-element method can be understood, as well as certain discretized versions of the integral equations describing scattering phenomena.

Finally, it is remarked that both forward (direct) and inverse modeling are natural consequences of the reciprocity theorem (cf. De Hoop [**7**]). Through an analysis of the type presented here, it is, at least theoretically, feasible that the whole operation of arriving at numerical results of a predetermined accuracy can be computer controlled.

2. THE ELASTODYNAMIC WAVE FIELD IN THE CONFIGURATION

The configuration in which the elastodynamic wave field is present consists of a solid material that occupies three-dimensional space R^3. In the bounded subdomain $D^s \subset R^3$ the solid is, in general, inhomogeneous and anisotropic. The boundary surface ∂D^s of D^s is assumed to be piecewise smooth. In the unbounded domain D_0 that is the complement of $D^s \cup \partial D^s$ in R^3, the solid is homogeneous and isotropic.

The position of observation in the configuration is specified by the coordinates $\{x_1, x_2, x_3\}$ with respect to a fixed, orthogonal, Cartesian reference frame with origin O and the three mutually perpendicular base vectors $\{\mathrm{i}_1, \mathrm{i}_2, \mathrm{i}_3\}$ of unit length each. In the indicated order, the base vectors form a right-handed system. The subscript notation for Cartesian vectors and tensors is used and the summation convention applies. The corresponding lowercase Latin subscripts are to be assigned the values $\{1, 2, 3\}$. Whenever appropriate, the position vector will be denoted by $\mathbf{x} = x_m \mathrm{i}_m$. The time coordinate is denoted by t. Partial differentiation is denoted by ∂; ∂_m denotes differentiation with respect to x_m, ∂_t is a reserved symbol for differentiation with respect to t.

For any causal space-time function $u = u(\mathbf{x}, t)$ the one-sided Laplace transform is introduced as

$$\hat{u}(\mathbf{x}, s) = \int_{t=0}^{\infty} \exp(-st) u(\mathbf{x}, t) dt, \tag{1}$$

where the instant $t = 0$ marks the onset of the events. Obviously, for bounded $\mid u(\mathbf{x}, t) \mid$, $\hat{u}(\mathbf{x}, s)$ is an analytic function of the complex transform parameter s in the right half $\mathrm{Re}(s) > 0$ of the complex s-plane. For ease of notation the circumflex over a symbol denoting its s-domain counterpart will be omitted in the remainder of the paper. The elastodynamic wave motion is started from a configuration at rest; then, under the one-sided Laplace transformation the operator ∂_t is replaced by an algebraic factor s.

In each subdomain of the configuration where the solid's acoustic properties vary continuously with position, the elastodynamic wave field quantities are continuously differentiable and satisfy the s-domain equations

$$-\Delta_{k,m,p,q} \partial_m \tau_{p,q} + s \rho_{k,r} v_r = f_k, \tag{2}$$

$$\Delta_{i,j,m,r} \partial_m v_r - s S_{i,j,p,q} \tau_{p,q} = h_{i,j}, \tag{3}$$

in which $\tau_{p,q}$ is the stress, v_r is the particle velocity, $\rho_{k,r}$ is the volume density of mass, $S_{i,j,p,q}$ is the compliance, f_k is the volume source density of force, and $h_{i,j}$ is the volume source density of rate of deformation. Full anisotropy in the inertia and (visco-)elastic properties of the solid is taken into account. For lossy solids (i.e., solids with relaxation), $\rho_{k,r}$ and $S_{i,j,p,q}$ are s-dependent, subject to the condition of causality which entails analyticity in $\mathrm{Re}(s) > 0$. Across interfaces between different kinds of solids (which are assumed to be in rigid contact), v_r and $\Delta_{k,m,p,q} \nu_m \tau_{p,q}$ are continuous, where ν_m is the unit vector to the normal along such an interface. The symmetrical unit tensor of rank four

$$\Delta_{k,m,p,q} = (1/2)(\delta_{k,p}\delta_{m,q} + \delta_{k,q}\delta_{m,p}), \tag{4}$$

where $\delta_{k,p}$ is the symmetrical unit tensor of rank two (Kronecker tensor), is characteristic for elastodynamics and automatically selects from any tensor of rank two with which it is contracted, the symmetrical part. In the configuration, objects can be present that are impenetrable to the elastodynamic wave motion. On the boundary surface of such an object explicit boundary conditions hold; admissible ones are: either $\Delta_{k,m,p,q}\nu_m\tau_{p,q} \rightarrow 0$ (void) or $v_r \rightarrow 0$ (immovable rigid object).

In the domain D_0 we have $\rho_{k,r} = \rho_0\delta_{k,r}$ and $S_{i,j,p,q} = \Lambda_0\delta_{i,j}\delta_{p,q} + 2M_0\Delta_{i,j,p,q}$, in which ρ_0, Λ_0 and M_0 are position independent. The elastodynamic wave field quantities that are generated by known sources in such a solid are analytically known (cf. Achenbach [8], De Hoop [9]). In deriving the relevant representations causality plays, again, an essential role.

3. THE RECIPROCITY RELATION

For our further analysis, the s-domain reciprocity relation that is associated with Eqs.(2) and (3) will serve as point of departure. A general wave field reciprocity theorem interrelates, in a specific manner, the quantities that characterize two different physical states that could occur in one and the same domain in space-time. For time-invariant configurations the application of the one-sided Laplace transformation of Eq.(1) to the convolution-type reciprocity theorem leads to an equivalent s-domain result. For this to be applicable to the configuration under investigation, the solids in the two states should be present in one and the same time-invariant domain D. The two states will be distinguished by the superscripts A and B, respectively.

First, the local reciprocity theorem will be derived. From it, the global reciprocity theorem for the entire configuration (or a subdomain of it) will be obtained. The local reciprocity relation follows upon considering the interaction quantity $\Delta_{k,m,p,q}\partial_m(\tau^A_{p,q}v^B_k - \tau^B_{p,q}v^A_k)$ and evaluating this quantity with the use of Eqs.(2) and (3) for the States A and B, respectively. The result is

$$\begin{aligned}\Delta_{k,m,p,q}\partial_m(\tau^A_{p,q}v^B_k - \tau^B_{p,q}v^A_k) \;=\; & s(\rho^A_{k,r} - \rho^B_{r,k})v^A_r v^B_k - s(S^A_{i,j,p,q} - S^B_{p,q,i,j})\tau^A_{p,q}\tau^B_{i,j} \\ & - f^A_k v^B_k + f^B_r v^A_r + h^B_{p,q}\tau^A_{p,q} - h^A_{i,j}\tau^B_{i,j}. \qquad (5)\end{aligned}$$

Equation (5) holds at any point of D in the neighborhood of which the properties of the solids in the States A and B vary continuously with position. As far as the right-hand side of Eq.(5) is concerned, the terms fall into two categories. In the first set of terms, the medium properties of the solids in the States A and B occur. These terms terms vanish if $\rho^A_{k,r} = \rho^B_{r,k}$ and $S^A_{i,j,p,q} = S^B_{p,q,i,j}$. If these properties hold, the solid present in State B is denoted as the adjoint of the solid present in State A. In case these properties hold for one and the same solid, this solid is denoted as self-adjoint or reciprocal. The second set of terms at the right-hand side is associated with the source distributions in the States A and B. Obviously, these terms vanish in a sourcefree subdomain.

The global reciprocity relation that holds for some domain D in the configuration is obtained by integrating Eq.(5) over the domain D and applying Gauss' divergence theorem to the resulting left-hand side. With this, the following relation is obtained:

$$\begin{aligned}&\int_{\partial D}\Delta_{k,m,p,q}\nu_m(\tau^A_{p,q}v^B_k - \tau^B_{p,q}v^A_k)dA \\ &= \int_D[s(\rho^A_{k,r} - \rho^B_{r,k})v^A_r v^B_k - s(S^A_{i,j,p,q} - S^B_{p,q,i,j})\tau^A_{p,q}\tau^B_{i,j} \\ &- f^A_k v^B_k + f^B_r v^A_r + h^B_{p,q}\tau^A_{p,q} - h^A_{i,j}\tau^B_{i,j}]dV, \qquad (6)\end{aligned}$$

where the contributions from interfaces have canceled in view of the pertaining boundary conditions of the continuity type, while the contributions from the boundary surfaces of impenetrable objects have vanished in view of the pertaining boundary conditons of the explicit type. Equation (6) is the global reciprocity relation that will be used in the considerations that follow. In it, ∂D is the boundary surface of the domain D and ν_m is the unit vector along its normal, pointing away from D.

In some of the applications, D will be the entire three-dimensional space. To address this situation, Eq. (6) is first applied to the domain interior to the sphere S_Δ of radius Δ and with center at the origin of the chosen reference frame, after which the limit $\Delta \rightarrow \infty$

is taken. From some Δ onward, S_Δ will be entirely situated in a homogeneous, isotropic, perfectly elastic solid. On S_Δ, the far-field representations for the elastodynamic wave field quantities can, for sufficiently large values of Δ, be used, from which the contribution from S_Δ can be shown to vanish in the limit $\Delta \to \infty$ (cf. De Hoop [**10**]).

4. DISCRETIZATION PROCEDURE AND ERROR CRITERIA

Each quantity $Q = Q(\mathbf{x}, s)$ occurring in the elastodynamic wave problem (be it a scalar, a vector, or a tensor of arbitrary rank) and defined on some domain D has, after discretization, a discretrized counterpart $[Q] = [Q](\mathbf{x}, s)$ defined on the discretized version $[D]$ of D. The local error δQ in Q is defined as

$$\delta Q(\mathbf{x}, s) = [Q](\mathbf{x}, s) - Q(\mathbf{x}, s) \quad \text{for } \mathbf{x} \in [D] \cap D. \tag{7}$$

The global error $ERR_\Omega(Q)$ in Q over some domain Ω is given by

$$ERR_\Omega(Q) = ERROP_\Omega(\delta Q), \tag{8}$$

where $ERROP$ is some positive definite operator acting on δQ over the domain Ω. For example, the root-mean-square error is given by

$$ERR_\Omega(Q) = RMS_\Omega(\delta Q), \tag{9}$$

where

$$RMS_\Omega(\delta Q) = \left[\int_{\mathbf{x}\in\Omega} \|\delta Q(\mathbf{x}, s)\|^2 dV\right]^{1/2}, \tag{10}$$

in which $\|\cdot\|$ denotes a suitably defined norm over Ω. Equation (8) defines the absolute global error in the quantity Q over the domain Ω. The relative global error $err_\Omega(Q)$ is taken as

$$err_\Omega(Q) = ERROP_\Omega(\delta Q)/ERROP_\Omega(Q). \tag{11}$$

Obviously, $err_\Omega(Q) = 0$ if $\delta Q = 0$ for all $\mathbf{x} \in \Omega$, and $err_\Omega(Q) = 1$ if $\delta Q = -Q$ for all $\mathbf{x} \in \Omega$.

Discretization of the computational domain

The actual machine computations are finite in number and can therefore only be carried out for some bounded computational domain $D \in R^3$. In the scheme to be presented, the inhomogeneous part D^s of the configuration has to be entirely incorporated in D, so we take D^s to be a proper subset of D. Note that the elastodynamic wave motion is defined in the entire R^3, which implies that D also contains some part of D_0, where the solid is homogeneous and isotropic. Without loss of generality we can therefore take the discretized version of the domain of computation identical to the actual one, i.e. $[D] = D$. Owing to this, the error analysis can be carried out over D, since both the exact and the discretized wave field quantities are then defined over D.

We now discretize D by taking it to be the union of a finite number of tetrahedra (simplices in R^3) that all have vertices, edges and faces in common. For any bounded domain, such a discretization can be carried out up to an error $O(h)$ as $h \to 0$, where h is the supremum of the maximum diameters of the tetrahedra (see, Naber [**11**]). The vertices of the tetrahedra will also be denoted as the nodes of the (geometrical) mesh and h will be denoted as the mesh size. Each quantity $Q = Q(\mathbf{x}, s)$ occurring in the elastodynamic wave field problem (be it a scalar, a vector, or a tensor of arbitrary rank) will, in the interior of each tetrahedron, be approximated by the linear interpolation of its values at the vertices. Let $\{\mathbf{x}(0), \mathbf{x}(1), \mathbf{x}(2), \mathbf{x}(3)\}$ denote the position vectors of the vertices of a particular tetrahedron (simplex) $SMPLX$, then the corresponding linear interpolation is given by

$$[Q](\mathbf{x}, s) = \sum_{IV=0}^{3} Q(IV, s)\lambda(IV; \mathbf{x}) \quad \text{for } \mathbf{x} \in SMPLX, \tag{12}$$

in which

$$Q(IV, s) = [Q](\mathbf{x}(IV), s), \quad \text{for } IV = 0, 1, 2, 3, \tag{13}$$

is the value of Q at the vertex with ordinal number IV, and $\{\lambda(IV; \mathbf{x}); IV = 0, 1, 2, 3\}$ are the barycentric coordinates of $\mathbf{x}$ in $SMPLX$. The latter have the property

$$\lambda(IV, \mathbf{x}(JV)) = \{1, 0\} \quad \text{if } \{IV = JV, IV \neq JV\}, \tag{14}$$

and are expressed in terms of the vectorial areas of the faces of $SMPLX$ through

$$\lambda(IV;\mathbf{x}) = 1/4 - (1/3V)(x_m - b_m)A_m(IV) \quad \text{with } IV = 0,1,2,3, \tag{15}$$

where $A_m(IV)$ is the outwardly oriented vectorial area of the face opposite the vertex with ordinal number IV and $b_m = (x_m(0) + x_m(1) + x_m(2) + x_m(3))/4$ is the position vector of the barycenter of $SMPLX$.

Discretization of the medium parameters

In the discretization of the medium parameters a distinction must be made between subdomains in which these parameters vary continuously with position and subdomains in which surfacess of discontinuity in these parameters occur. It is assumed that across such surfaces of discontinuity in medium parameters, the parameter values jump by finite amounts. Especially in applications where accurate values of the wave field quantities up to these surfaces are needed (such as, for example, in the modeling of borehole measurement situations in exploration geophysics, and for applications in the non-destructive evaluation of mechanical structures), special measures have to be taken to model accurately the behavior of these quantities. In principle, the medium properties are allowed to jump across any face of any tetrahedron of the discretized geometry. To accomodate this feature, all nodes of the geometrical mesh are considered as multiple nodes, where the multiplicity of each node is equal to the number of tetrahedra that meet at that node. The values of the constitutive parameters at the vertices that are needed in the local expansion Eq.(12), follow either from user-supplied input expressions that are spatially sampled in the interior of each tetrahedron close to each of its vertices (as is the case in direct or forward profiling problems) or from computationally derived values (as is the case in inverse profiling problems). Out of the thus constructed local expansions of the medium parameters, their global expansions over the domain of computation are composed by combining the local expansions. If in the latter procedure, at a particular node no discontinuity turns up, the multiple node is changed into a simple one, with an associated single value of the relevant constitutive parameter. For the non-scalar constitutive parameters the components with respect to the background Cartesian reference frame are used in the entire discretization procedure.

Discretization of the volume source densities

For the discretization of the volume source densities the same procedure as for the discretization of the medium parameters is followed.

Discretization of the wave field quantities

In the discretization of the elastodynamic wave field quantities the situation is more complicated. Here, some components are by necessity continuous across an interface of discontinuity in material properties, while other components show a finite jump across such a discontinuity surface. To preserve accuracy in the computational results, it is necessary, both in the modeling of direct or forward problems and in the modeling of inverse problems, to take computational measures that enforce the continuity conditions across an interface (in machine precision) and leave the non-continuous components free to jump by finite amounts. For this purpose, local expansions of the type of Eq.(12) have been developed where a non-scalar quantity at a vertex is expressed in terms of its components that are continuous across an interface of discontinuity in material properties. These components are, in general, not the components with respect to the background Cartesian reference frame. For the elastodynamic wave field quantities the relevant difficulty does not arise in connection with the particle velocity: all components of this quantity are continuous across the interfaces of discontinuity in material properties, since we have assumed the two media at either side of each interface to be in rigid contact. For the stress, however, the components normal to an interface (that together form the traction) are continuous across the interface, while the remaining components show a jump discontinuity. To guarantee the continuity of the traction across each face of adjoining tetrahedra, we consider each node as a multiple node and construct at each vertex the stress out of the three tractions at the three faces that meet at that vertex and use the relevant values in the local expansion Eq.(12). The relevant elements are denoted as face elements. Out of the thus constructed local expansions, the global expansions over the domain of computation are composed by combining the local expansions. If in this procedure simple nodes are met, the stress is just expressed in terms of

its components in the background Cartesian reference frame. The face-element representation for the global expansion of the stress could also be used at simple nodes, but this leads to an unnecessarily large number of expansion coefficients to be computed (without yielding an increased accuracy) since the number of tetrahedral faces that meet at a particular node is larger than three.

5. FINITE-ELEMENT MODELING

To construct the system of equations that results from the finite-element modeling of elastodynamic wave problems, we apply the global Betti-Rayleigh reciprocity relation Eq.(6) to the discretized computational domain $[D]$, substitute the proper expansions for State A in it, put the constitutive coefficients for State B equal to zero, and successively take for the wave field in State B one of the global expansion functions of State A, while at the boundary surface $\partial[D]$ of the domain of computation an 'absorbing' boundary condition is invoked.

6. INTEGRAL-EQUATION MODELING

To construct the system of equations that results from the integral-equation modeling of elastodynamic wave problems, we apply the global Betti-Rayleigh reciprocity relation Eq.(6) to the discretized computational domain $[D]$, substitute the proper expansions for State A into it, put the constitutive coefficients for State B equal to the ones of the embedding D_0, and successively take for the sources in State B one of the global expansions of State A. (In this way we construct, in fact, the discretized Green's functions of the embedding.)

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