WAVE MOTION 12 (1990) 67–80
NORTH-HOLLAND

THEORETICAL CONSIDERATIONS ON A FINITE-ELEMENT METHOD FOR THE COMPUTATION OF THREE-DIMENSIONAL SPACE-TIME ELASTODYNAMIC WAVE FIELDS

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Received 4 July 1988

The theory of a space-time finite-element method for the numerical solution of elastodynamic wave problems in bounded time-invariant subdomains of three-dimensional space is developed. It is shown how the finite-element method can be regarded as to be based on a space-time elastodynamic reciprocity theorem of the time-correlation type. Particular local representations for the elastodynamic wave field (particle velocity and stress) are introduced that can handle strongly inhomogeneous structures with solid/solid, fluid/fluid and fluid/solid interfaces.

1. Introduction

The theoretical essentials of a full space-time finite-element method, based on reciprocity considerations, for the numerical solution of elastodynamic wave problems in bounded, time-invariant subdomains of three-dimensional space are developed. The configuration may consist of fluid and solid parts. The wave fields in the fluid parts are characterized by their particle velocity and scalar traction; the wave fields in solid parts are characterized by their particle velocity and stress; these quantities are regarded as the state variables. It is shown how the finite-element method can be regarded as to be based on a space-time elastodynamic reciprocity theorem of the time-correlation type [1]. In its turn this theorem is shown to be equivalent to a certain weighting procedure applied to the equation of motion and the deformation rate equation that govern the wave motion. The fluids and solids in the configuration are taken to be linear, locally and instantaneously reacting, and time-invariant in their elastic behavior. Arbitrary inhomogeneity and anisotropy are taken into account. Particular local representations for the acoustic and elastodynamic wave field quantities are proposed that can handle strongly inhomogeneous structures, in which solid/solid, fluid/fluid and fluid/solid interfaces may be present.

2. Basic equations of elastodynamics

The acoustic/elastodynamic waves under consideration are small-amplitude mechanical disturbances that propagate in a time-invariant configuration in three-dimensional space. Position of observation in R^3 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 $\{\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3\}$ of unit length each. In the indicated order the base vectors form a right-handed system. The subscript notation for Cartesian vectors and tensors in R^3 is employed and the summation convention applies. The corresponding lower-case

Latin subscripts are to be assigned the values $\{1, 2, 3\}$. Whenever appropriate, the position vector will be denoted by the bold-face symbol $\boldsymbol{x} = x_p \boldsymbol{i}_p$. The time coordinate is denoted by t. Partial differentiation is denoted by ∂; ∂_p denotes differentiation with respect to x_p, ∂_t denotes differentiation with respect to t. SI-units are used throughout.

The geometrical configuration that we study is taken to be time-invariant. The fluids and solids present in it are assumed to be linear, locally and instantaneously reacting, and time-invariant in their elastic behavior. They may be arbitrarily inhomogeneous and anisotropic. Let the configuration occupy the bounded domain $D \subset R^3$, and let D^s be the subdomain occupied by the solid and D^f the subdomain occupied by the fluid. The boundary of D is denoted by ∂D; the part of ∂D in the fluid is denoted by S^f and the part of ∂D in the solid by S^s (see Fig. 1). In D^s we characterize the elastodynamic wave field of the configuration by its particle velocity v_r and its stress τ_{pq}, while the physical properties of the solid are characterized by its tensorial volume density of mass ρ_{kr} (see [2]) and its compliance s_{ijpq}. In each subdomain of D^s where the elastodynamic properties vary continuously with position, the elastodynamic wave field quantities are continuously differentiable and satisfy the (linearized) equation of motion [3, p. 55], [4, p. 85], [5, p. 17]

$$-\Delta_{kmpq}\partial_m \tau_{pq} + \rho_{kr}\partial_t v_r = f_k, \tag{2.1}$$

and the (linearized) deformation rate equation

$$\Delta_{ijmr}\partial_m v_r - s_{ijpq}\partial_t \tau_{pq} = h_{ij}, \tag{2.2}$$

where f_k = volume source density of force, h_{ij} = volume density of strain rate and $\Delta_{kmpq} = (\delta_{kp}\delta_{mq} + \delta_{kq}\delta_{mp})/2$ is a unit tensor of rank four that specifically occurs in elastodynamics (δ_{kp} is the Kronecker tensor: $\delta_{kp} = 1$ if $k = p$ and $\delta_{kp} = 0$ if $k \neq p$); it has the symmetry properties $\Delta_{kmpq} = \Delta_{mkpq} = \Delta_{mkqp} = \Delta_{qpmk}$. At an interface between two different solids the constitutive coefficients ρ_{kr} and s_{ijpq} in general jump by finite amounts. In all applications we shall assume that at a solid/solid interface the media are in rigid contact; then, the particle velocity and the traction are continuous across the interface, i.e., at each point $\boldsymbol{x}$ of a solid/solid interface we have (Fig. 2)

$$\lim_{h \uparrow 0} v_r(\boldsymbol{x} + \boldsymbol{\nu} h) = \lim_{h \downarrow 0} v_r(\boldsymbol{x} + \boldsymbol{\nu} h) \quad \text{and} \quad \lim_{h \uparrow 0} t_k(\boldsymbol{x} + \boldsymbol{\nu} h) = \lim_{h \downarrow 0} t_k(\boldsymbol{x} + \boldsymbol{\nu} h), \tag{2.3-2.4}$$

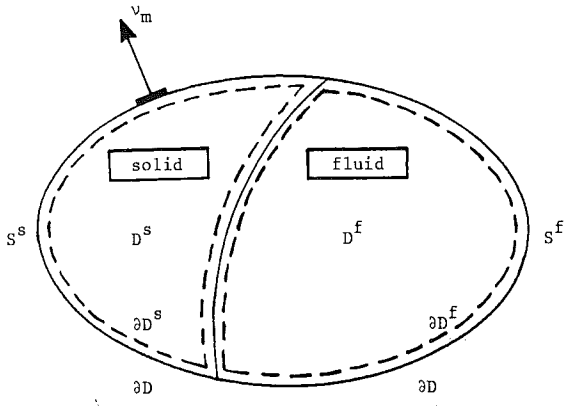

Fig. 1. Domain D consisting of the subdomains D^s and D^f with closed outer boundary ∂D and its outwardly directed unit normal vector ν_m. The part of ∂D adjacent to the solid is denoted by S^s and the part of ∂D adjacent to the fluid by S^f; ∂D^s is the closed boundary of D^s, ∂D^f is the closed boundary of D^f.

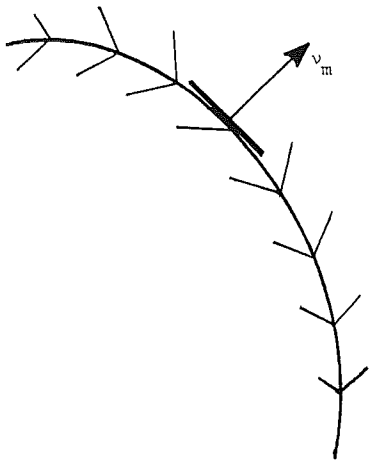

Fig. 2. Interface with unit normal vector ν.

where t_k is the traction, defined as $t_k = \Delta_{kmpq}\nu_m\tau_{pq}$, and $\boldsymbol{\nu} = \nu_m \boldsymbol{i}_m$ is the unit vector along the normal to the solid/solid interface at the point $\boldsymbol{x}$.

The acoustic wave field in D^f is characterized by its particle velocity v_r and its scalar traction σ (the opposite of the pressure). The physical properties of the fluid are characterized by its tensorial volume density of mass ρ_{kr} (see [6]) and its compressibility κ. In each subdomain of D^f where the acoustic properties vary continuously with position, the acoustic wave field quantities are continuously differentiable and satisfy the (linearized) equation of motion [7, p. 4]

$$-\delta_{km}\partial_m\sigma + \rho_{kr}\partial_t v_r = f_k, \tag{2.5}$$

and the (linearized) deformation rate equation

$$\delta_{mr}\partial_m v_r - \kappa\partial_t\sigma = q, \tag{2.6}$$

where f_k = volume source density of force, q = volume density of injection rate. Although (2.5) and (2.6) could be written in a simpler manner ($\delta_{km}\partial_m = \partial_k$), we have retained in the first term on the left-hand side the Kronecker tensor for reasons of symmetry with the elastodynamic equations. At an interface between two different fluids the constitutive coefficients ρ_{kr} and κ in general jump by finite amounts. Across a fluid/fluid interface the normal component of the particle velocity and the scalar traction are continuous, i.e., at each point $\boldsymbol{x}$ of a fluid/fluid interface we have (Fig. 2)

$$\lim_{h\uparrow 0} \nu_r v_r(\boldsymbol{x}+\boldsymbol{\nu}h) = \lim_{h\downarrow 0} \nu_r v_r(\boldsymbol{x}+\boldsymbol{\nu}h) \quad \text{and} \quad \lim_{h\uparrow 0} \sigma(\boldsymbol{x}+\boldsymbol{\nu}h) = \lim_{h\downarrow 0} \sigma(\boldsymbol{x}+\boldsymbol{\nu}h), \tag{2.7-2.8}$$

where $\boldsymbol{\nu} = \nu_m \boldsymbol{i}_m$ is the unit vector along the normal to the fluid/fluid interface at the point $\boldsymbol{x}$.

The last type of interface that can occur in the configuration is a fluid/solid interface. Across a fluid/solid interface the normal component of the particle velocity is continuous and the normal component of the fluid traction equals the normal component of the solid traction, while the tangential component of the solid traction is equal to zero, i.e., at each point $\boldsymbol{x}$ of a fluid/solid interface we have (Fig. 2)

$$\lim_{h\uparrow 0} \nu_r v_r(\boldsymbol{x}+\boldsymbol{\nu}h) = \lim_{h\downarrow 0} \nu_r v_r(\boldsymbol{x}+\boldsymbol{\nu}h), \qquad \lim_{h\uparrow 0} \nu_k t_k(\boldsymbol{x}+\boldsymbol{\nu}h) = \lim_{h\downarrow 0} \sigma(\boldsymbol{x}+\boldsymbol{\nu}h), \tag{2.9-2.10}$$

and

$$\lim_{h\uparrow 0} t_k(\boldsymbol{x}+\boldsymbol{\nu}h) - \nu_k\nu_q t_q(\boldsymbol{x}+\boldsymbol{\nu}h) = 0, \tag{2.11}$$

where $\boldsymbol{\nu} = \nu_m \boldsymbol{i}_m$ is the unit vector along the normal to the fluid/solid interface at the point $\boldsymbol{x}$ pointing away from the solid.

To account for causality in the wave problem, we need initial conditions at some instant $t = t_0$ after which the sources are considered to act; these are denoted by

$$v_r(\boldsymbol{x}, t_0) = v_r^{\mathrm{I}}(\boldsymbol{x}), \quad \text{and} \quad \tau_{pq}(\boldsymbol{x}, t_0) = \tau_{pq}^{\mathrm{I}}(\boldsymbol{x}) \quad \text{when } \boldsymbol{x} \in D^{\mathrm{s}} \tag{2.12}$$

and

$$v_r(\boldsymbol{x}, t_0) = v_r^{\mathrm{I}}(\boldsymbol{x}), \quad \text{and} \quad \sigma(\boldsymbol{x}, t_0) = \sigma^{\mathrm{I}}(\boldsymbol{x}) \quad \text{when } \boldsymbol{x} \in D^{\mathrm{f}}. \tag{2.13}$$

Further, we need boundary conditions at the boundary surface ∂D of D. In a number of applications these are of the explicit type. The admissible ones are shown in Table 1 (Fig. 3).

With these boundary conditions, the initial/boundary-value problem can be shown to have a unique solution. The proof runs along the same way as the uniqueness of the solution of the elastodynamic wave problem in a solid [3, pp. 80–82], [4, pp. 176–177], [5, p. 24].

In many scattering problems a certain strongly inhomogeneous configuration is considered to be embedded in a so-called 'invariant embedding' [8] whose properties are taken to be relatively simple ones (for example, homogeneous and isotropic), such that the Green's functions (point-excitation solutions to the wave problem) can be constructed analytically. If this model applies, the contrast-source formulation of the inhomogeneities with respect to the embedding leads to non-local boundary conditions on ∂D that manage the scattered wave to radiate into the embedding. The corresponding initial/boundary-value problem can, in this case, too, be shown to have a unique solution. Combined with the finite-element

Table 1

The admissible explicit boundary conditions on ∂D

Part of exterior boundary surface	Adjacent to	Prescribed value of	Type of problem
S_1^{f}	fluid	normal velocity	Dirichlet
S_2^{f}	fluid	scalar traction	Neumann
S_1^{s}	solid	velocity	Dirichlet
S_2^{s}	solid	traction	Neumann

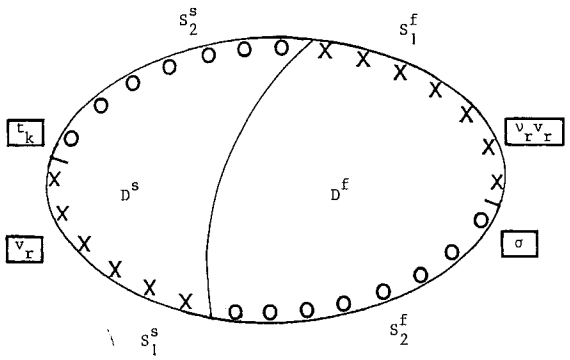

Fig. 3. The four types of explicit boundary conditions prescribed at the different parts of the outer boundary ∂D; ××× = Dirichlet, ○○○ = Neumann.

method applied to the inhomogeneous domain D, the corresponding computational method is known as the hybrid-element method [9, 10].

3. The space-time finite element method

As the starting point for setting up a finite-element formulation of the acoustic wave problem we take the space-time elastodynamic reciprocity theorem of the time-correlation type [1]. A reciprocity theorem interrelates in a specific way two physical states that could be present in one and the same domain. In the realm of our wave problem we have a relation between two elastodynamic wave fields. We distinguish their state quantities by the superscripts A and B. In our application of the theorem the Field A is identified with the actual wave field that is to be computationally approximated, while the Field B is considered as a computational one that remains to be chosen appropriately. It is noted that the computational Field B need not represent a physical elastodynamic wave field, but only has to satisfy the equations (2.1) and (2.2) in D^s and (2.5) and (2.6) in D^f. As regards the space-time geometry in which the two states occur, the time-invariance implies that this geometry is the Cartesian product $D \times R$ of a time-invariant spatial domain $D \subset R^3$ and the real time axis R. For the elastodynamic waves in the solid parts, the theorem is applied to the bounded subdomain D^s of D where the solid medium is present. Let the latter consist of the subdomains $\{D^{s,N};\ N = 1, \ldots, N^s\}$ where the medium properties vary continuously with position. Hence the state quantities are continuously differentiable in $\{D^{s,N};\ N = 1, \ldots, N^s\}$. Let the closed boundary surface of $D^{s,N}$ be denoted by $\partial D^{s,N}$ (Fig. 4), then the required reciprocity relation is

$$\begin{aligned}
&\sum_{N=1}^{N^s} \int_{t\in R} \mathrm{d}t \int_{x\in\partial D^{s,N}} \Delta_{mrpq}\nu_m[v_r^{\mathrm{A}}(\boldsymbol{x},t)\tau_{pq}^{\mathrm{B}}(\boldsymbol{x},t-\tau)+v_r^{\mathrm{B}}(\boldsymbol{x},t-\tau)\tau_{pq}^{\mathrm{A}}(\boldsymbol{x},t)]\,\mathrm{d}A \\
&\quad=\partial_\tau \int_{t\in R} \mathrm{d}t \int_{x\in D^s} \tau_{ij}^{\mathrm{B}}(\boldsymbol{x},t-\tau)[s_{ijpq}^{\mathrm{A}}(\boldsymbol{x})-s_{pqij}^{\mathrm{B}}(\boldsymbol{x})]\tau_{pq}^{\mathrm{A}}(\boldsymbol{x},t)\,\mathrm{d}V \\
&\quad+\partial_\tau \int_{t\in R} \mathrm{d}t \int_{x\in D^s} v_k^{\mathrm{B}}(\boldsymbol{x},t-\tau)[\rho_{kr}^{\mathrm{A}}(\boldsymbol{x})-\rho_{rk}^{\mathrm{B}}(\boldsymbol{x})]v_r^{\mathrm{A}}(\boldsymbol{x},t)\,\mathrm{d}V \\
&\quad+\int_{t\in R} \mathrm{d}t \int_{x\in D^s} \tau_{ij}^{\mathrm{B}}(\boldsymbol{x},t-\tau)h_{ij}^{\mathrm{A}}(\boldsymbol{x},t)-v_k^{\mathrm{B}}(\boldsymbol{x},t-\tau)f_k^{\mathrm{A}}(\boldsymbol{x},t)\,\mathrm{d}V \\
&\quad+\int_{t\in R} \mathrm{d}t \int_{x\in D^s} \tau_{pq}^{\mathrm{A}}(\boldsymbol{x},t)h_{pq}^{\mathrm{B}}(\boldsymbol{x},t-\tau)-v_r^{\mathrm{A}}(\boldsymbol{x},t)f_r^{\mathrm{B}}(\boldsymbol{x},t-\tau)\,\mathrm{d}V. \qquad (3.1)
\end{aligned}$$

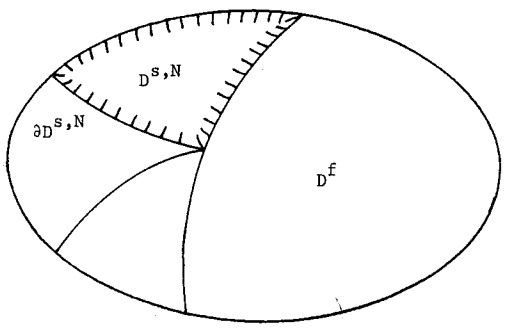

Fig. 4. Domain D^s consisting of the subdomains $\{D^{s,N};\ N = 1, 2, \ldots, N^s\}$ with boundaries $\partial D^{s,N}$.

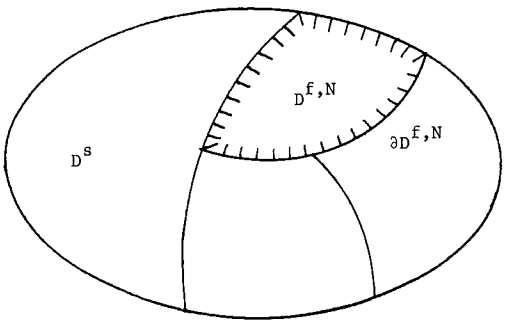

Fig. 5. Domain D^f consisting of the subdomains $\{D^{f,N};\ N = 1, 2, \ldots, N^f\}$ with boundaries $\partial D^{f,N}$.

First of all we shall show that equation (3.1) can, from a particular point of view, be regarded as a 'weighted' form of the equation of motion (2.1) and the deformation rate equation (2.2) pertaining to the State A. To this end, we take the quantities $\{v_k^B, \tau_{ij}^B\}$ of the computational State B to be continuously differentiable in each of the subdomains $\{D^{s,N}; N=1,\ldots,N^s\}$, while we take $\rho_{rk}^B=0$, $s_{pqij}^B=0$, $f_r^B=-\Delta_{rmij}\partial_m\tau_{ij}^B$ and $h_{pq}^B=\Delta_{pqmk}\partial_m v_k^B$. Substituting these quantities into (3.1) and applying Gauss' divergence theorem to each of the subdomains $\{D^{s,N}; n=1,\ldots,N^s\}$, of D^s, we end up with

$$\int_{t\in R} \mathrm{d}t \int_{x\in D^s} v_k^B(x,t-\tau)[-\Delta_{kmpq}\partial_m\tau_{pq}^A(x,t)+\rho_{kr}^A(x)\partial_t v_r^A(x,t)-f_k^A(x,t)]\,\mathrm{d}V$$
$$-\int_{t\in R} \mathrm{d}t \int_{x\in D^s} \tau_{ij}^B(x,t-\tau)[\Delta_{ijmr}\partial_m v_r^A(x,t)-s_{ijpq}^A(x)\partial_t\tau_{pq}^A(x,t)-h_{ij}^A(x,t)]\,\mathrm{d}V=0. \tag{3.2}$$

Upon now taking the functions $\tau_{ij}^B=0$ (and hence $f_r^B=0$) throughout $D^s\times R$, and $v_k^B\neq 0$, equation (3.2) amounts to the weighted form of the equation of motion (2.1) over the space-time domain $D^s\times R$ with the arbitrary weighting function v_k^B. If, on the other hand, we take the functions $v_k^B=0$ (and hence $h_{pq}^B=0$) throughout $D^s\times R$, and $\tau_{ij}^B\neq 0$, equation (3.2) amounts to the weighted form of the deformation rate equation (2.2) over the space-time domain $D^s\times R$ with the arbitrary weighting function τ_{ij}^B.

For the acoustic waves in the fluid parts, the theorem is applied to the bounded subdomain D^f of D where a fluid medium is present. Let the latter consist of subdomains $\{D^{f,N}; N=1,\ldots,N^f\}$ where the medium properties vary continuously with position and hence the state quantities are piecewise continuously differentiable in $\{D^{f,N}; N=1,\ldots,N^f\}$. Let the closed boundary surface of $D^{f,N}$ be denoted by $\partial D^{f,N}$ (Fig. 5), then the required reciprocity relation is

$$\sum_{N=1}^{N^f}\int_{t\in R}\mathrm{d}t\int_{x\in\partial D^{f,N}}\delta_{mr}\nu_m[v_r^A(x,t)\sigma^B(x,t-\tau)+v_r^B(x,t-\tau)\sigma^A(x,t)]\,\mathrm{d}A$$
$$=\partial_\tau\int_{t\in R}\mathrm{d}t\int_{x\in D^f}\sigma^B(x,t-\tau)[\kappa^A(x)-\kappa^B(x)]\sigma^A(x,t)\,\mathrm{d}V$$
$$+\partial_\tau\int_{t\in R}\mathrm{d}t\int_{x\in D^f}v_k^B(x,t-\tau)[\rho_{kr}^A(x)-\rho_{rk}^B(x)]v_r^A(x,t)\,\mathrm{d}V$$
$$+\int_{t\in R}\mathrm{d}t\int_{x\in D^f}\sigma^B(x,t-\tau)q^A(x,t)-v_k^B(x,t-\tau)f_k^A(x,t)\,\mathrm{d}V$$
$$+\int_{t\in R}\mathrm{d}t\int_{x\in D^f}\sigma^A(x,t)q^B(x,t-\tau)-v_r^A(x,t)f_r^B(x,t-\tau)\,\mathrm{d}V. \tag{3.3}$$

Equation (3.3) can, from a particular point of view, be regarded as a 'weighted' form of the equation of motion (2.5) and the deformation rate equation (2.6) pertaining to the State A. To show this, we take the quantities $\{v_k^B, \sigma^B\}$ of State B to be continuously differentiable in the subdomains $\{D^{f,N}; N=1,\ldots,N^f\}$, while we take $\rho_{rk}^B=0$, $\kappa^B=0$, $f_r^B=-\delta_{rm}\partial_m\sigma^B$ and $q^B=\delta_{mk}\partial_m v_k^B$. Substituting these quantities into (3.3) and using Gauss' divergence theorem in the subdomains $\{D^{f,N}; N=1,\ldots,N^f\}$ of D^f where both sides are continuously differentiable, we end up with

$$\int_{t\in R}\mathrm{d}t\int_{x\in D^f}v_k^B(x,t-\tau)[-\delta_{km}\partial_m\sigma^A(x,t)+\rho_{kr}^A(x)\partial_t v_r^A(x,t)-f_k^A(x,t)]\,\mathrm{d}V$$
$$-\int_{t\in R}\mathrm{d}t\int_{x\in D^f}\sigma^B(x,t-\tau)[\delta_{mr}\partial_m v_r^A(x,t)-\kappa^A(x)\partial_t\sigma^A(x,t)-q^A(x,t)]\,\mathrm{d}V=0. \tag{3.4}$$

Upon now taking the function $\sigma^B = 0$ (and hence $f_r^B = 0$) throughout $D^f \times R$, and $v_k^B \neq 0$, equation (3.4) amounts to the weighted form of the equation of motion (2.5) over the space-time domain $D^f \times R$ with the arbitrary weighting function v_k^B. If, on the other hand, we choose the functions $v_k^B = 0$ (and hence $q^B = 0$) throughout $D^f \times R$, and $\sigma^B \neq 0$, equation (3.4) amounts to the weighted form of the deformation rate equation (2.6) over the space-time domain $D^f \times R$ with the arbitrary weighting function σ^B.

The formulations (3.2) and (3.4) are now used to set up a space-time finite-element method. In these formulations the Field A is identified with an approximation to the actual wave field and the Field B with an appropriate weighting field within the category discussed above. Upon taking a reciprocity relation as the point of departure of setting up a numerical scheme, it seems more or less natural to treat the States A and B in an equivalent manner, which implies that each specimen of the sequence of functions into which State A is expanded is also taken as a specimen of the State B. As far as (3.2) and (3.4) are concerned, this implies that the sequence of weighting functions is taken to be the same as the sequence of expansion functions. This procedure leads to a system of linear algebraic equations with the expansion coefficients of State A as the unknowns. Boundary conditions of the explicit type are accounted for by prescribing those expansion coefficients that are related to the relevant field values of State A at the boundary of D. The above method is known as the method of weighted residuals ([11, pp. 38–39], [12, pp. 287–306], [13, pp. 138–139]).

To model an acoustic/elastodynamic wave field that radiates into an exterior unbounded domain where the Green's function is known, non-local acoustic boundary conditions are applied. These boundary conditions relate the wave field quantities at the boundary ∂D to their values in the interior of D via the pertaining (discretized) source-type integral representations. In the solution of the wave problem these relations are added to the equations that follow from using the finite-element method for the interior field in D.

4. The local expansion functions

In this section particular local expansion functions are introduced that are used to approximate the acoustic and elastodynamic wave field. In view of the time-invariance of the domain D of computational interest, the space-time domain over which the finite-element method is applied, is discretized into a union of elementary subdomains that are cylindrical in the time direction. Their maximum diameter in space is denoted as the mesh size of the discretization. In these subdomains local expansion functions to represent the field quantities are defined that are the product of a function of the spatial variables and a function of time. In conjunction with the cylindricity of the space-time domain in the time direction, this leads to two independent discretizations: one in the spatial direction and one in the direction of time. In our discussion we shall concentrate on the spatial discretization because in this direction inhomogeneities may occur. The simplest local interpolation function is the polynomial of degree zero, i.e., a constant in each elementary subdomain of the configuration; the value of this constant is attributed to the wave field value at the barycenter of the elementary subdomain. The corresponding piecewise constant interpolation of the wave field quantities in the spatial direction has the disadvantage that all components of the represented wave field quantities are discontinuous across the boundaries of the subdomains, which physically implies that spurious surface-source distributions of the order of the mesh size of the geometrical discretization are introduced, with an accompanying error in the field values. To avoid this inaccuracy, polynomial expansion functions of degree one are taken; they are the lowest-degree polynomials by which physically non-existing surface source distributions on interfaces of discontinuity can numerically be avoided in the representations. At the same time, they are the ones through which a consistent interpolation

is achieved in the most fundamental geometrical shape (the simplex [14, p. 49]), all spatial directions being treated alike. For the expansion functions in time no restrictions follow from the reciprocity theorem of Section 3. However, we can argue that for the description of wave motions, where the time and spatial coordinates play an equivalent role, linear time expansion functions are the most suited ones in combination with the linear spatial expansion functions.

To arrive at the desired linear interpolation functions, the spatial domain is discretized into a union of tetrahedra the vertices of which coincide with the nodes of the spatial discretization and the time axes is discretized into a union of intervals the edge points of which coincide with the nodes of the time discretization. The position vectors of the four vertices $\{P(0), P(1), P(2), P(3)\}$ of a representative tetrahedron T are denoted by $\{x_i(0), x_i(1), x_i(2), x_i(3)\}$, respectively. The position in the interior of T or on its boundary ∂T can be specified by the barycentric coordinates $\{\lambda(0), \lambda(1), \lambda(2), \lambda(3)\}$ defined through

$$x_i = \sum_{I=0}^{3} \lambda(I)\, x_i(I), \quad \text{with } 0 \leqslant \lambda(I) \leqslant 1 \text{ and } \sum_{I=0}^{3} \lambda(I) = 1. \tag{4.1}$$

We observe that the barycentric coordinates $\lambda(I)$ do perform the linear interpolation in the tetrahedron (viz. of the position vector) we are looking for. To express them in terms of x_i, some geometrical quantities associated with T are needed. First, the vectorial areas $\{A_i(0), A_i(1), A_i(2), A_i(3)\}$ of the faces of T that are directed along the outward normals to the faces of T are introduced; they are given by (for the numbering we refer to Fig. 6)

$$\begin{aligned}
A_i(0) &= \varepsilon_{ijk}\frac{x_j(1)x_k(2)+x_j(2)x_k(3)+x_j(3)x_k(1)}{2},\\
A_i(1) &= -\varepsilon_{ijk}\frac{x_j(2)x_k(3)+x_j(3)x_k(0)+x_j(0)x_k(2)}{2},\\
A_i(2) &= \varepsilon_{ijk}\frac{x_j(3)x_k(0)+x_j(0)x_k(1)+x_j(1)x_k(3)}{2},\\
A_i(3) &= -\varepsilon_{ijk}\frac{x_j(0)x_k(1)+x_j(1)x_k(2)+x_j(2)x_k(0)}{2},
\end{aligned} \tag{4.2}$$

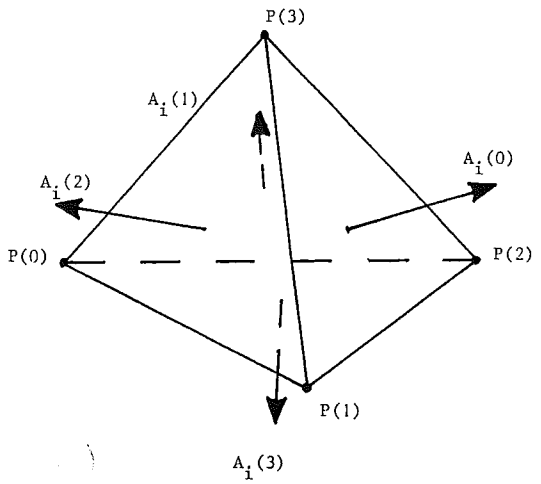

Fig. 6. Tetrahedron T with its four vertices $\{P(0), P(1), P(2), P(3)\}$ and the outwardly directed vectorial areas $\{A_i(0), A_i(1), A_i(2), A_i(3)\}$ of its faces.

where ε_{ijk} is the completely antisymmetric unit tensor of rank three (Levi-Civita tensor). It follows that

$$\sum_{I=0}^{3} A_i(I) = 0. \tag{4.3}$$

The volume of T is given by

$$V = \varepsilon_{ijk} \frac{-x_i(0)x_j(1)x_k(2) + x_i(1)x_j(2)x_k(3) - x_i(2)x_j(3)x_k(0) + x_i(3)x_j(0)x_k(1)}{6}. \tag{4.4}$$

Now, we observe that at each vertex of T, the three vectorial edges leaving that vertex and the three vectorial areas of the faces meeting at that vertex form, apart from a constant factor, a set of (oblique) reciprocal base vectors. Let us consider the vertex $P(0)$. The three vectorial edges leaving this vertex are $\{x_i(1) - x_i(0), x_i(2) - x_i(0), x_i(3) - x_i(0)\}$ and the three vectorial areas of the faces meeting at this vertex are $\{A_i(1), A_i(2), A_i(3)\}$. Now, it is easily verified that

$$[x_i(I) - x_i(0)]\, A_i(J) = -3V\delta(I, J), \quad \text{with } I = 1, 2, 3 \text{ and } J = 1, 2, 3, \tag{4.5}$$

where $\delta(I, I) = 1$ and $\delta(I, J) = 0$ if $I \neq J$. From (4.5) it follows that, at the vertex with position vector $x_i(0)$, the set of vectors $\{-[x_i(1) - x_i(0)]/3V, -[x_i(2) - x_i(0)]/3V, -[x_i(3) - x_i(0)]/3V\}$ is reciprocal to the set $\{A_i(1), A_i(2), A_i(3)\}$, and the set $\{-A_i(1)/3V, -A_i(2)/3V, -A_i(3)/3V\}$ is reciprocal to the set $\{x_i(1) - x_i(0), x_i(2) - x_i(0), x_i(3) - x_i(0)\}$. Returning to (4.1), we can, by letting $\lambda(0) = 1 - \lambda(1) - \lambda(2) - \lambda(3)$, write

$$x_i - x_i(0) = \sum_{I=1}^{3} \lambda(I)[x_i(I) - x_i(0)]. \tag{4.6}$$

Upon multiplying this equation by $-(3V)^{-1}A_i(J)$ and using (4.5) we obtain

$$-(3V)^{-1}[x_i - x_i(0)]\, A_i(J) = \lambda(J) \quad \text{for } J = 1, 2, 3. \tag{4.7}$$

Since further, on account of (4.3),

$$-(3V)^{-1}[x_i - x_i(0)]\, A_i(0) = -\sum_{I=1}^{3} \lambda(I), \tag{4.8}$$

it follows that

$$x_i - x_i(0) = -(3V)^{-1} \sum_{J=0}^{3} [x_j - x_j(0)]\, A_j(J)\, x_i(J). \tag{4.9}$$

Similar results hold for the other vertices as well. By combining the results we have

$$x_i - x_i(I) = -(3V)^{-1} \sum_{J=0}^{3} [x_j - x_j(I)]\, A_j(J)\, x_i(J) \quad \text{for } I = 0, 1, 2, 3. \tag{4.10}$$

Summing the results for $I = 0, 1, 2, 3$, respectively, and introducing the position vector b_i of the barycenter of T through

$$b_i = \tfrac{1}{4} \sum_{I=0}^{3} x_i(I), \tag{4.11}$$

we arrive at the symmetrical expression

$$x_i = b_i - (3V)^{-1} \sum_{I=0}^{3} (x_j - b_j)\, A_j(I)\, x_i(I). \tag{4.12}$$

On account of this relation, we can write

$$x_i = \sum_{I=0}^{3} x_i(I)\, \phi(I; \boldsymbol{x}), \tag{4.13}$$

where

$$\phi(I; \boldsymbol{x}) = \tfrac{1}{4} - (3V)^{-1}(x_j - b_j)\, A_j(I). \tag{4.14}$$

Comparing (4.13) with (4.1), we see that $\{\phi(I; \boldsymbol{x});\ I = 0, 1, 2, 3\}$ are nothing but the barycentric coordinates of a point in T or on its boundary ∂T. On the other hand, $\phi(I; \boldsymbol{x})$ performs a linear scalar interpolation between the value one at the vertex $x_i = x_i(I)$ and zero at the remaining vertices of T.

The positions of the edge points $T(0)$ and $T(1)$ of a representative interval TIM on the discretized time axes are denoted by $t(0)$ and $t(1)$. In each interval TIM two local interpolation functions are defined by

$$\psi(M, t) = (t - t(N))/(t(M) - t(N)), \quad M = 0, 1,\ N \neq M. \tag{4.15}$$

The function $\psi(M, t)$ performs a linear interpolation between the value one at the edge point $t = t(M)$ and zero at the remaining edge point.

In the following, the local functions $\phi(I; \boldsymbol{x})$, defined on $T \cup \partial T$ and $\psi(M, t)$, defined on TIM, are employed to interpolate the particle velocity v_r in the solid and the fluid, the scalar traction σ in the fluid and the stress τ_{pq} in the solid in the tetrahedron T. Let $\{\sigma(I; M), v_r(I; M), \tau_{pq}(I; M),\ I = 0, 1, 2, 3;\ M = 0, 1\}$ denote the values of $\{\sigma, v_r, \tau_{pq}\}$ when $x_i = x_i(I)$ is approached via the interior of T and $t = t(M)$ is approached via the interior of TIM, then their local representations are

$$\{\sigma(\boldsymbol{x}, t), v_r(\boldsymbol{x}, t), \tau_{pq}(\boldsymbol{x}, t)\} = \sum_{I=0}^{3} \sum_{M=0}^{1} \{\sigma(I; M), v_r(I; M), \tau_{pq}(I; M)\}\phi(I; \boldsymbol{x})\psi(M; t)$$

$$\text{for } (\boldsymbol{x}, t) \in \{T \cup \partial T\} \times \text{TIM}. \tag{4.16}$$

In the representation (4.16) the choice of how at each vertex the vectors $v_r(I; M)$ and the tensors $\tau_{pq}(I; M)$ are decomposed is still open. This choice is determined by the physics of the problem, in particular by whether the nodal point with which the vertex coincides either is or is not on an interface, and if yes, what type of interface (fluid/fluid, fluid/solid, solid/solid) it is. For each of these cases the appropriate choice will be discussed in Section 5.

In the discretized geometry we take the elastodynamic properties of the medium and the volume source densities to be linearly varying with position in each tetrahedral subdomain of D and the surface sources are taken to be linearly varying on each triangular subdomain of the discretized outer boundary ∂D of the domain of computational interest.

5. Choice of the vectorial/tensorial decompositions at the vertices of a tetrahedron

The different possibilities that occur in an inhomogeneous fluid/solid configuration and the choices of how vectors and tensors at a vertex of a tetrahedral subdomain of the configuration are to be composed will be discussed separately below.

Vertex coincides with nodal point not on an interface

In a vertex that coincides with a nodal point that is not on an interface we decompose the field quantities along the axes of the background Cartesian reference frame.

Vertex coincides with nodal point on a solid/solid interface

Across a solid/solid interface all components of the particle velocity and the normal component of the stress (the traction) are to be continuous, while the tangential components of the stress may jump by finite amounts. Accordingly, in a vertex $x_i(I)$ of a tetrahedron T that coincides with a nodal point located on a solid/solid interface, the particle velocity is decomposed along the axes of the background Cartesian reference frame, and the stress $\tau_{pq}(I; M)$ is written as

$$\tau_{pq}(I; M) = -(3V)^{-1} \sum_{J=0}^{3} T_p(I, J; M)[x_q(J) - x_q(I)], \tag{5.1}$$

i.e., as far as its second subscript is concerned it is decomposed along the local base vectors $\{-(3V)^{-1}[x_q(J) - x_q(I)],\ J = 0, 1, 2, 3,\ J \neq I\}$ that are directed along the edges meeting in $x_i(I)$. Using (4.5), it follows that the expansion coefficient

$$T_p(I, J; M) = \tau_{pq}(I; M)\, A_q(J), \quad \text{with } I \neq J, \tag{5.2}$$

is the traction at the face with vectorial area $A_q(J)$ in the vertex $x_i(I)$ at the instant $t(M)$ times the area of the face. Obviously, the term with $J = I$ drops automatically from the summation (5.1); for later purposes it is, however, advantageous to put

$$T_p(I, I; M) = 0. \tag{5.3}$$

Vertex coincides with nodal point on a fluid/fluid interface

Across a fluid/fluid interface the normal components of the particle velocity are continuous while the tangential components of the particle velocity may jump by finite amounts. Accordingly, in each vertex $x_i(I)$ of a tetrahedron T that coincides with a nodal point that is located on a fluid/fluid interface the particle velocity $v_r(I; M)$ is written as

$$v_r(I; M) = -(3V)^{-1} \sum_{J=0}^{3} V(I, J; M)[x_r(J) - x_r(I)]. \tag{5.4}$$

i.e., it is decomposed along the local base vectors $\{-(3V)^{-1}[x_r(J) - x_r(I)],\ J = 0, 1, 2, 3,\ J \neq I\}$ that are directed along the edges meeting in $x_i(I)$. Using (4.5) it follows that the expansion coefficient

$$V(I, J; M) = v_r(I; M)\, A_r(J) \quad \text{with } J \neq I \tag{5.5}$$

is the normal component of the particle velocity at the face with vectorial area $A_r(J)$ in the vertex $x_i(I)$ at the time $t(M)$ times the area of the face. Obviously, the term with $J = I$ drops automatically from the summation in (5.4); for later purposes it is, however, advantageous to put

$$V(I, I; M) = 0. \tag{5.6}$$

It is noted that for the scalar traction σ the expansion (4.16) holds.

Vertex coincides with nodal point on a fluid/solid interface

Across a fluid/solid interface the normal component of the particle velocity is continuous while its tangential component may jump by finite amounts. Further, the normal component of the traction in the solid is equal to the scalar traction in the fluid, while the tangential components of the traction in the solid are equal to zero. Accordingly, in a vertex $x_i(I)$ of a tetrahedron T that coincides with a nodal point that is located on a fluid/solid interface the particle velocity $v_r(I; M)$ is represented by (5.4) and the stress $\tau_{pq}(I; M)$ by (5.1) where the coefficient $T_p(I, J; M)$ is now given as

$$T_p(I, J; M) = -(3V)^{-1} \sum_{K=0}^{3} T(I, J, K; M)[x_p(K) - x_p(I)]. \tag{5.7}$$

i.e., the stress is completely decomposed along the local base vectors $\{-(3V)^{-1}[x_p(K) - x_p(I)],\ K = 0, 1, 2, 3,\ K \neq I\}$ that are directed along the edges meeting in $x_i(I)$. Using (4.5) it follows that the expansion coefficient is given by

$$T(I, J, K; M) = T_p(I, J; M)\, A_p(K) \quad \text{with } J \neq I,\ K \neq I. \tag{5.8}$$

Substitution of (5.7) into (5.1) gives the representation of the stress $\tau_{pq}(I; M)$ in the vertex $x_i(I)$ at the instant $t(M)$:

$$\tau_{pq}(I; M) = (3V)^{-2} \sum_{J=0}^{3} \sum_{K=0}^{3} T(I, J, K; M)[x_p(K) - x_p(I)][x_q(J) - x_q(I)]. \tag{5.9}$$

For $K = J$ the coefficient (5.8) is the normal component of the traction at the face with vectorial area $A_p(J)$ in $x_i(I)$ at the instant $t(M)$ times the square of the area of the face. Obviously, the terms with $K = I$ and $J = I$ in (5.9) drop from the summation. It is advantageous however, to put

$$T(I, I, K; M) = T(I, J, I; M) = 0. \tag{5.10}$$

With this, for nodal points located on either of the interfaces under consideration, appropriate expansions for the elastodynamic state quantities have been defined.

6. Global spatial expansion functions

Now that in Section 5 the different local expansion functions have been constructed, we are able to construct the corresponding global expansion functions. In this, we let ourselves guide by the same type of argument as that has been used in [15] for the representation of three-dimensional electromagnetic fields for finite-element modeling in strongly inhomogeneous media, i.e., we want functions that (in the computer code automatically) guarantee the continuity of all field-components that are continuous across an interface, while leaving the non-continuous components free to jump by finite amounts. In the realm of acoustic and elastodynamic wave fields this implies that near interfaces we construct representations for the fields that automatically satisfy the interface conditions (2.3), (2.4) and (2.7)–(2.11) while leaving the remaining components free to jump by finite amounts.

The set of expansion coefficients that follows upon allocating to each tetrahedron of the discretized geometry the local expansions of Section 5 is now introduced as the set of 'vertex' expansion coefficients, each vertex being considered as a 'multiple node' of the grid that covers the domain of computational interest, with multiplicity equal to the number of tetrahedra that have the particular vertex in common (i.e., that form the simplicial star of that vertex). If now, depending on the location of the vertex (not on

an interface, or on a solid/solid, fluid/fluid, or fluid/solid interface) it follows from the physics that some or all of the vertex expansion coefficients of a multiple node should have equal values, this common vertex expansion coefficient is introduced as a single nodal expansion coefficient. Thus, the number of nodal expansion coefficients is (sometimes considerably) less than the number of vertex expansion coefficients. The set of nodal expansion coefficients is next introduced as the set of global expansion coefficients and correspondingly the global expansion functions are introduced as the ones that have as spatial support the union of all tetrahedra to which the particular global expansion coefficient applies and that perform the linear interpolation from the value one at the node under consideration to the value zero at the remaining nodes of its support. In this manner the global expansion of the acoustic wave field satisfies (again, in the computer code automatically) the continuity and jump requirements at each of the interfaces present in the domain of computational interest.

With this philosophy as regards the spatial expansion functions a finite-element code is under development.

7. Conclusion

The theory of a space-time finite-element method for the numerical computation of three-dimensional elastodynamic wave motions in bounded, time-invariant configurations that may be anisotropic and strongly inhomogeneous, is presented. It is shown that the finite-element method can be considered to be based on a space-time reciprocity theorem of the time-correlation type. Linear spatial expansions for the representation of the particle velocity in the fluid and the solid, the stress in the solid and the scalar traction in the fluid in the discretized geometry are constructed that automatically guarantee the continuity requirements at interfaces of discontinuity in material properties (solid/solid, fluid/fluid, fluid/solid) in an elastic configuration while leaving noncontinuous elastodynamic field components free to jump by finite amounts. For these functions as spatial elementary subdomain the tetrahedron was taken. In the time direction, piecewise linear functions in combination with the linear spatial functions were considered as the most suited ones to describe in a consistent way wavelike phenomena.

Acknowledgement

The research presented in this paper has been sponsored by Royal/Dutch Shell Exploration and Production Laboratories, Rijswijk, The Netherlands. This financial support is gratefully acknowledged.

References

[1] A.T. de Hoop and H.J. Stam, "Time-domain reciprocity theorems for elastodynamic wave fields in solids with relaxation and their application to inverse problems", *Wave Motion 10*, 479–489 (1988).
[2] T.J.I'A. Bromwich, "Note on the wave surface of a dynamical medium, aeolotropic in all respects", *Proc. London Math. Soc. 34*, 307–321 (1902).
[3] J.D. Achenbach, *Wave Propagation in Elastic Solids*, North-Holland, Amsterdam (1973).
[4] A.E.H. Love, *A Treatise on the Mathematical Theory of Elasticity*, Cambridge University Press, Cambridge (1959), 4th ed.
[5] K. Aki and P.G. Richards, *Quantitative Seismology*, Freeman, San Francisco (1980).
[6] Lord Rayleigh, "On double refraction", *Scientific Papers 1*, Cambridge University Press, Cambridge (1899) 111–119.
[7] H. Lamb, *Hydrodynamics*, Cambridge University Press, Cambridge (1957), 6th ed.

[8] R. Bellman and R. Kalaba, "On the principle of invariant imbedding and propagation through inhomogeneous media", *Proc. Nat. Acad. Sci. U.S.A. 42*, 629–632 (1956).
[9] K.H. Lee, D.F. Pridmore and H.F. Morrison, "A hybrid three-dimensional electromagnetic modeling scheme", *Geophysics 46*, 796–805 (1981).
[10] P.K. Gupta, L.A. Bennett and A.P. Raiche, "Hybrid calculations of the three-dimensional electromagnetic response of buried conductors", *Geophysics 52*, 301–306 (1987).
[11] O.C. Zienkiewicz, *The Finite Element Method in Engineering Science*, McGraw-Hill, London (1971).
[12] J.N. Reddy, *Applied Functional Analysis and Variational Methods in Engineering*, McGraw-Hill, New York (1986).
[13] G. Dhatt and G. Touzot, *The Finite Element Method Displayed*, Wiley, New York (1984).
[14] L. Naber, *Topological Methods in Euclidian Spaces*, Cambridge University Press, Cambridge (1980).
[15] G. Mur and A.T. de Hoop, "A finite-element method for computing three-dimensional electromagnetic fields in inhomogeneous media", *IEEE Trans. Magnetics 21*, 2188–2191 (1985).