Finite differences at structural interfaces

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Summary

Proposed is the method of designing the finite–difference schemes of the 2^{nd} and 4^{th} order in 2-D and 3-D regular rectangular grids, both inside geological blocks and at structural interfaces. Considered are only the point schemes, expressed in terms of the gridpoint values of the material and other model parameters and of the wavefield. The common, simple, and highly symmetric point schemes are applicable only in smooth parts of seismic models, inside geological blocks. To maintain the comparable accuracy at structural interfaces, special finite–difference schemes have to be derived. These special schemes are linear operators acting on the wavefield gridpoint values, and are dependent on the positions and slopes of the interfaces.

Keywords

Finite differences of the 2^{nd} and 4^{th} order, 2-D and 3-D seismic modelling, structural interfaces, elasticity, anisotropy.

1 Introduction

In this paper, proposed is the method of designing the finite–difference schemes of the 2^{nd} and 4^{th} order in 2-D and 3-D regular rectangular grids, both inside geological blocks and at structural interfaces. Considered are only the point schemes, expressed in terms of the gridpoint values of the material and other model parameters and of the wavefield.

In Sections 2 and 3, the method of designing the point finite–difference schemes applicable in smooth parts of seismic models, outside structural interfaces, is presented. The method is suitable both in isotropic and anisotropic seismic models. The schemes have a general form of linear operators acting on the wavefield gridpoint values, and represent the common, simple, and highly symmetric point schemes applicable only in smooth parts of seismic models, inside geological blocks.

To maintain the comparable accuracy at structural interfaces, special finite–difference schemes have to be derived. Fortunately, the point finite–difference schemes may be generalized for the application in the vicinity of structural interfaces, by means of wavefield matching at the interfaces. The principles of the wavefield matching at structural interfaces are outlined in Section 4.

The general form of the final special finite–difference schemes, accurately applicable at structural interfaces, is given in Section 5. These special schemes are linear operators acting on the wavefield gridpoint values, and are dependent on the positions and slopes of the interfaces. These linear operators should be evaluated before starting a finite–difference calculation, and their coefficients should be stored in the memory. The number of the coefficients of each linear operator equals the number of wavefield components (2 in 2-D, or 3 in 3-D) times the number of gridpoints on which the scheme is dependent. The recommended number of these gridpoints is 9 or 25 for the 2-D finite differences of the 2^{nd} or 4^{th} order, respectively, and 19 or 65 for the 3-D finite differences of the

2^{nd} or 4^{th} order, respectively. The storage of the coefficients of all schemes crossing structural interfaces (i.e. of all schemes dependent on the gridpoints from different geological blocks) requires some amount of computer random access memory. On the other hand, the application of these special schemes does not noticeably slow down the finite–difference calculation.

Finally, Section 6 outlines how to deal with free space.

This paper does not deal with the boundary conditions at the boundaries of the model volume covered by the rectangular grid. Thus the theory derived applies only to the inner gridpoints of a rectangular grid of points.

Throughout the paper, the model is assumed to be composed of "sufficiently smooth" geological blocks separated by a set of "sufficiently smooth" interfaces. Here "sufficiently smooth" is understood, above all, with respect to the grid density. The grid interval h is assumed to be sufficiently smaller than the characteristic lengths L of the inhomogeneities inside geological blocks, and simultaneously sufficiently smaller than the radii R of curvature of structural interfaces. These conditions are, as the author believes, the natural requirements for model gridding.

2 Wavefield on a rectangular grid

2.1 Gridpoint values

At a time level, the wavefield is represented by gridpoint values $u_i(\mathbf{x})$, where the positional vector $\mathbf{x}$ takes the values (positions) of all gridpoints. In the computer memory, the gridpoints are, as a rule, indexed. Then the positional vector $\mathbf{x}$ is represented by the corresponding integer index, and $u_i(\mathbf{x})$ by an array.

Let us denote by $\mathbf{h}_i$ the vectorial grid intervals. If the grid is regular and rectangular in the Cartesian coordinates, and the grid interval in all directions is of the same length h, we may choose

$$\mathbf{h}_1 = (h,0,0)^{\mathrm{T}} \ , \quad \mathbf{h}_2 = (0,h,0)^{\mathrm{T}} \ , \quad \mathbf{h}_3 = (0,0,h)^{\mathrm{T}} \quad . \tag{1}$$

The gridpoints $\mathbf{y}$, from the vicinity of fixed gridpoint $\mathbf{x}$ situated inside the grid, may then be expressed in the form of

$$\mathbf{y} = \mathbf{x} + n_1\mathbf{h}_1 + n_2\mathbf{h}_2 + n_3\mathbf{h}_3 = \mathbf{x} + n_i\mathbf{h}_i \quad , \tag{2}$$

where n_1, n_2, and n_3 are small signed integers. For instance, $n_i = -1, 0, 1$ for 3-D finite differences of the second order, and $n_I = -1, 0, 1$, $n_3 = 0$ for 2-D finite differences of the second order. If the gridpoints are indexed, grid intervals $\mathbf{h}_1$, $\mathbf{h}_2$, $\mathbf{h}_3$ are represented by the corresponding shifts of the index. For example, if the grid values in the grid of dimensions $5 \times 4 \times 3$ are stored in the Fortran manner, $\mathbf{h}_1 = 1$, $\mathbf{h}_2 = 5$, and $\mathbf{h}_3 = 20$ in the computer representation.

2.2 Taylor expansion

For fixed gridpoint $\mathbf{x}$ situated inside the grid, we denote

$$u_{i(n_1,n_2,n_3)} = u_i(\mathbf{x} + n_1\mathbf{h}_1 + n_2\mathbf{h}_2 + n_3\mathbf{h}_3) \quad . \tag{3}$$

These grid values are the arguments of a linear finite–difference operator. Within the smooth geological block, the grid values may be approximated by the Taylor expansion from gridpoint $\mathbf{x}$.

Let us denote by

$$\begin{aligned} &U_i = u_i(\mathbf{x}) \ , \quad U_{ij} = u_{i,j}(\mathbf{x}) = \frac{\partial u_i}{\partial x_j}(\mathbf{x}) \ , \quad U_{ijk} = u_{i,jk}(\mathbf{x}) = \frac{\partial^2 u_i}{\partial x_j \partial x_k}(\mathbf{x}) \ , \\ &U_{ijkl} = u_{i,jkl}(\mathbf{x}) = \frac{\partial^3 u_i}{\partial x_j \partial x_k \partial x_l}(\mathbf{x}) \ , \\ &U_{ijklm} = u_{i,jklm}(\mathbf{x}) = \frac{\partial^4 u_i}{\partial x_j \partial x_k \partial x_l \partial x_m}(\mathbf{x}) \ , \quad \dots \quad . \end{aligned} \tag{4}$$

the value and partial derivatives of the wavefield at $\mathbf{x}$. Then the gridpoint values (3) may be approximated by

$$u_{i(n_1,n_2,n_3)} = U_i + hU_{ij}n_j + \frac{h^2}{2}U_{ijk}n_jn_k + \frac{h^3}{6}U_{ijkl}n_jn_kn_l + \frac{h^4}{24}U_{ijklm}n_jn_kn_ln_m + \dots \ . \tag{5}$$

We arrange, for fixed $\mathbf{x}$, the grid values (3) into vector $\mathbf{u}$, and the partial derivatives (4) into vector $\mathbf{U}$. Equal derivatives (e.g. U_{112} and U_{121}) are summed to form a single element of $\mathbf{U}$ (e.g. $U_{1[12]} = U_{112} + U_{121}$, where index $[i,j]$ corresponds to all permutations of i and j). Then the Taylor expansion (5) may be expressed as the linear transformation

$$\mathbf{u} = \mathbf{T}\mathbf{U} \quad , \tag{6}$$

where the elements of the Taylor–expansion matrix $\mathbf{T}$, projecting U_i, U_{ij}, $U_{i[jk]}$, $U_{i[jkl]}$, $U_{i[jklm]}$, ... onto $u_{n(n_1,n_2,n_3)}$, are

$$\begin{aligned} &T_{n(n_1,n_2,n_3):i} = \delta_{ni} \ , \\ &T_{n(n_1,n_2,n_3):ij} = \delta_{ni} h n_j \ , \\ &T_{n(n_1,n_2,n_3):i[jk]} = \delta_{ni}\frac{h^2}{2}n_jn_k \ , \\ &T_{n(n_1,n_2,n_3):i[jkl]} = \delta_{ni}\frac{h^3}{6}n_jn_kn_l \ , \\ &T_{n(n_1,n_2,n_3):i[jklm]} = \delta_{ni}\frac{h^4}{24}n_jn_kn_ln_m \ , \quad \dots \quad . \end{aligned} \tag{7}$$

2.3 Second time derivatives of the wavefield

Let us consider general linear stress–strain relations

$$\sigma_{ij} = c_{ijkl} u_{k,l} \quad , \tag{8}$$

where c_{ijkl} are the elastic parameters. In an isotropic medium,

$$c_{ijkl} = \delta_{ij}\delta_{kl}\lambda + \delta_{ik}\delta_{jl}\mu + \delta_{il}\delta_{jk}\mu \quad , \tag{9}$$

where

$$\lambda = \varrho({v_{\mathrm{P}}}^2 - 2{v_{\mathrm{S}}}^2) \; , \quad \mu = \varrho {v_{\mathrm{S}}}^2 \quad . \tag{10}$$

The second partial time derivative of the wavefield is then

$$u_{i,tt} = \varrho^{-1}\frac{\partial \sigma_{ij}}{\partial x_j} = \varrho^{-1}(c_{ijkl}u_{k,lj} + c_{ijkl,j}u_{k,l}) \quad , \tag{11}$$

and specifically at $\mathbf{x}$

$$u_{i,tt}(\mathbf{x}) = \varrho^{-1}(C_{ijkl}U_{klj} + C_{ijklj}U_{kl}) \quad , \tag{12}$$

where

$$C_{ijkl} = c_{ijkl}(\mathbf{x}) \; , \quad C_{ijklm} = \frac{\partial c_{ijkl}}{\partial x_m}(\mathbf{x}) \tag{13}$$

are the values and partial derivatives of the elastic parameters at central point $\mathbf{x}$. In an isotropic medium,

$$C_{ijkl}U_{klj} = (\lambda + \mu)\,U_{kki} + \mu U_{ikk} \quad , \tag{14}$$

$$C_{ijklj} = \delta_{kl}\frac{\partial \lambda}{\partial x_i}(\mathbf{x}) + \delta_{il}\frac{\partial \mu}{\partial x_k}(\mathbf{x}) + \delta_{ik}\frac{\partial \mu}{\partial x_l}(\mathbf{x}) \quad , \tag{15}$$

and

$$C_{ijklj}U_{kl} = \frac{\partial \lambda}{\partial x_i}(\mathbf{x})\; U_{kk} + \frac{\partial \mu}{\partial x_k}(\mathbf{x})\; [U_{ik} + U_{ki}] \quad . \tag{16}$$

Partial derivatives C_{ijklm} of the elastic parameters at $\mathbf{x}$ may be estimated using symmetrical differences

$$C_{ijklm} = \frac{1}{2h}[c_{ijkl}(\mathbf{x} + \mathbf{h}_m) - c_{ijkl}(\mathbf{x} - \mathbf{h}_m)] \tag{17}$$

of the second order if all points $\mathbf{x} - \mathbf{h}_m$, $\mathbf{x}$, $\mathbf{x} + \mathbf{h}_m$ are situated in the same geological block. In other words, if the points are not separated by a structural interface. At structural interfaces, partial derivatives C_{ijklm} should preferably be calculated by the model–specification software instead of differencing.

Equation (12) is the linear dependence

$$\mathbf{t} = \mathbf{S}\mathbf{U} \tag{18}$$

of the vector

$$\mathbf{t} = (u_{1,tt}, u_{2,tt}, u_{3,tt})^{\mathrm{T}} \tag{19}$$

on the vector $\mathbf{U}$ of the partial derivatives. The only non–zero components of the matrix $\mathbf{S}$ are

$$S_{n\;ij} = \varrho^{-1}C_{ijnkk} \; , \quad S_{n\;ijk} = \varrho^{-1}(C_{ijkn} + C_{ikjn})/2 \quad , \tag{20}$$

projecting U_{ij} and $U_{i[jk]}$ onto $u_{n,tt}$, respectively.

3 Finite–difference schemes inside geological blocks

To determine the finite–difference scheme, we select N wavefield values at the gridpoints within the vicinity of each central point $\mathbf{x}$. These N values determine vector $\mathbf{u}$ of wavefield grid values. Equation (6) then represents N linear equations for the partial wavefield derivatives ordered in vector $\mathbf{U}$. We thus have to select N non–zero partial derivatives and put all other components of $\mathbf{U}$ equal zero. The partial wavefield derivatives up to the second order must not be annulled. The set of N non–zero components of $\mathbf{U}$ has to be selected in such a way that the resulting system (6) of N linear equations for N non–zero components of $\mathbf{U}$ is regular. Thus, in our approach, the finite–difference scheme will be fully determined by selecting the set of N gridpoint wavefield values (arguments of the scheme) and the set of N non–zero partial wavefield derivatives.

If choosing a reasonable subset $\mathbf{u}$ of grid values (3) and the corresponding reasonable subset $\mathbf{U}$ of partial derivatives (4), the Taylor–expansion matrix $\mathbf{T}$ may be inverted and equation (6) can be solved,

$$\mathbf{U} = \mathbf{T}^{-1}\mathbf{u} \quad . \tag{21}$$

From (7) it is obvious that inverse Taylor–expansion matrix $\mathbf{T}^{-1}$ is dependent only on the grid structure and on the selected size and structure of the vectors $\mathbf{u}$ and $\mathbf{U}$, i.e. on the choice of the finite–difference scheme. Moreover, for a regular grid, inverse Taylor–expansion matrix $\mathbf{T}^{-1}$ is the same for all "inner" gridpoints $\mathbf{x}$. The finite–difference schemes of "inner" gridpoints do not cross the grid boundaries or structural interfaces.

The finite–difference scheme inside a smooth geological block may now be expressed in the general matrix form of

$$\mathbf{t} = \mathbf{S}\mathbf{T}^{-1}\mathbf{u} \quad . \tag{22}$$

4 Wavefield matching at structural interfaces

Let us assume that the structural interface is smooth in the vicinity of gridpoint $\mathbf{x}$ and may be described in the parametric form of

$$y_i = y_i(\xi_1, \xi_2) \quad . \tag{23}$$

The Taylor expansion of (23) may be expressed in the form of

$$\begin{aligned} z_i(\xi_1,\xi_2) &= y_i(\xi_1,\xi_2) - x_i \\ &= Z_i + Z_{iJ}\xi_J + \frac{1}{2}Z_{iJK}\xi_J\xi_K + \frac{1}{6}Z_{iJKL}\xi_J\xi_K\xi_L + \frac{1}{24}Z_{iJKLM}\xi_J\xi_K\xi_L\xi_M + \dots \ , \end{aligned} \tag{24}$$

where we assume that the central point $x_i + Z_i$ of the interface expansion lies in the vicinity of the gridpoint x_i, i.e. approximately within the volume in which the gridpoints influencing the finite–difference scheme are situated. Then terms Z_i and $Z_{iJ}\xi_J$ are of the order of h, and term $\frac{1}{2}Z_{iJK}\xi_J\xi_K$ is of the order of h^2/R, where R is the curvature radius of the interface. Each subsequent term in (24) should be less significant than the preceding term by a factor of the order of h/R.

The following quantities has to be continuous across the interface:
(a) the wavefield

$$u_i(\xi_1,\xi_2) = U_i + U_{ij}z_j + \frac{1}{2}U_{ijk}z_jz_k + \frac{1}{6}U_{ijkl}z_jz_kz_l + \frac{1}{24}U_{ijklm}z_jz_kz_lz_m + \dots \ ; \tag{25}$$

(b) the traction

$$\sigma_{ij} n_j = c_{ijkl} n_j u_{k,l} \quad , \tag{26}$$

where

$$n_i(\xi_1, \xi_2) = N_i + N_{iJ}\xi_J + \frac{1}{2} N_{iJK}\xi_J\xi_K + \frac{1}{6} N_{iJKL}\xi_J\xi_K\xi_L + \dots \quad , \tag{27}$$

is the normal to the interface,

$$\begin{aligned}
[\sigma_{ij} n_j](\xi_1, \xi_2) = {} & C_{ijkl} n_j U_{kl} \\
& + [C_{ijkl} n_j U_{klm} + C_{ijklm} n_j U_{kl}] z_m \\
& + \frac{1}{2}[C_{ijkl} n_j U_{klmn} + 2C_{ijklm} n_j U_{kln} + C_{ijklmn} n_j U_{kl}] z_m z_n \\
& + \frac{1}{6}[C_{ijkl} n_j U_{klmnp} + 3C_{ijklm} n_j U_{klno} + 3C_{ijklmn} n_j U_{klp} + C_{ijklmnp} n_j U_{kl}] z_m z_n z_p \\
& + \dots ;
\end{aligned} \tag{28}$$

(c) the second derivative (11) of the wavefield with respect to time,

$$\begin{aligned}
u_{i,tt}(\xi_1, \xi_2) = {} & \varrho^{-1}[C_{ijkl} U_{klj} + C_{ijklj} U_{kl}] \\
& + \varrho^{-1}[C_{ijkl} U_{kljm} + (C_{ijklm} - \varrho^{-1}\varrho_{,m} C_{ijkl}) U_{klj} \\
& \quad + C_{ijklj} U_{klm} + (C_{ijkljm} - \varrho^{-1}\varrho_{,m} C_{ijklj}) U_{kl}] z_m \\
& + (2\varrho)^{-1}[C_{ijkl} U_{kljmn} + 2(C_{ijklm} - \varrho^{-1}\varrho_{,m} C_{ijkl}) U_{kljn} \\
& \quad + (C_{ijklmn} - 2\varrho^{-1}\varrho_{,m} C_{ijkln} + 2\varrho^{-2}\varrho_{,m}\varrho_{,n} C_{ijkl} - \varrho^{-1}\varrho_{,mn} C_{ijkl}) U_{klj} \\
& \quad + C_{ijklj} U_{klmn} + (C_{ijkljm} - \varrho^{-1}\varrho_{,m} C_{ijklj}) U_{kln} + \dots] z_m z_n + \dots ;
\end{aligned} \tag{29}$$

(d) the second derivative of the traction with respect to time

$$\begin{aligned}
\sigma_{ij,tt} n_j = {} & c_{ijkl} n_j (u_{k,tt})_{,l} \\
= {} & c_{ijkl} n_j [\varrho^{-1}(c_{kmnp} u_{n,pm} + c_{kmnpm} u_{n,p})]_{,l} \\
= {} & c_{ijkl} n_j \varrho^{-1}(c_{kmnp} u_{n,pml} + c_{kmnpl} u_{n,pm} \\
& \qquad - \varrho^{-1}\varrho_{,l} c_{kmnp} u_{n,pm} + c_{kmnpm} u_{n,pl} + \dots) \ ,
\end{aligned} \tag{30}$$

$$\begin{aligned}
[\sigma_{ij,tt} n_j](\xi_1, \xi_2) = {} & C_{ijkl} n_j \varrho^{-1}[C_{kmnp} U_{npml} + C_{kmnpl} U_{npm} \\
& \qquad - \varrho^{-1}\varrho_{,l} C_{kmnp} U_{npm} + C_{kmnpm} U_{npl} + \dots] \\
& + C_{ijkl} n_j \varrho^{-1}[C_{kmnp} U_{npmlq} + C_{kmnpq} U_{npml} + C_{kmnpl} U_{npmq} \\
& \qquad - \varrho^{-1}\varrho_{,l} C_{kmnp} U_{npmq} + C_{kmnpm} U_{nplq} + \dots] z_q + \dots ;
\end{aligned} \tag{31}$$

(e) the fourth derivative of the wavefield with respect to time

$$\begin{aligned}
u_{i,tttt} &= \varrho^{-1}\{c_{ijkl}[u_{k,tt}]_{,l}\}_{,j} \\
&= \varrho^{-1}\{c_{ijkl}[\varrho^{-1}(c_{kmnp} u_{n,p})_{,m}]_{,l}\}_{,j} \\
&= \varrho^{-2} c_{ijkl} c_{kmnp} u_{n,pmlj} + \dots \ ,
\end{aligned} \tag{32}$$

$$u_{i,tttt}(\xi_1,\xi_2) = [\varrho^{-2}C_{ijkl}C_{kmnp}U_{npmlj}+...]+[\varrho^{-2}C_{ijkl}C_{kmnp}U_{npmljq}+...]z_q+... \quad ; \quad (33)$$

(...) etc.

The principal terms in (28), (29), (31), (33) are the terms without derivatives of elastic parameters C_{ijkl} and ϱ. The principal terms with the 3^{rd}, 4^{th}, ... partial wavefield derivatives are of the orders of h/Λ, $(h/\Lambda)^2$, ... compared with the principal term containing the 2^{nd} partial wavefield derivatives. Here Λ denotes the wavelength. Neglecting these terms, we introduce the relative errors of the orders of h/Λ, $(h/\Lambda)^2$, ... in the propagation velocity at each interface. The corresponding errors of the travel time are of the orders of $h^2/(v\Lambda)$, $(h^3/(v\Lambda^2)$, ... at each interface. The corresponding relative errors in terms of amplitude, caused by a single interface, are then of the orders of $(h/\Lambda)^2$, $(h/\Lambda)^3$, ... Since h/Λ is often of the order of 1 for the shortest wavelengths, all the principal terms are meaningful.

The terms with the first partial derivatives C_{ijklm} or $C_{ijkl}\varrho_{,m}$ of the elastic parameters are, compared with the corresponding principal terms, of the order of Λ/L. Neglecting these terms, containing the 1^{st}, 2^{nd}, 3^{rd}, 4^{th}, ... wavefield derivatives, we introduce the relative errors of the orders of Λ/L, h/L, $h^2/(\Lambda L)$, $h^3/(\Lambda^2 L)$, ... in the propagation velocity at each interface. The corresponding errors of the travel time are of the orders of $h\Lambda/(vL)$, $h^2/(vL)$, $h^3/(v\Lambda L)$, $h^4/(v\Lambda^2 L)$, ... at each interface. The corresponding relative errors in terms of amplitude, caused by a single interface, are then of the orders of h/L, $h^2/(\Lambda L)$, $h^3/(\Lambda^2 L)$, $h^4/(\Lambda^3 L)$, ..., that should be negligible for most of reasonably discretized models.

The linear term $N_{iJ}\xi_J$ in (27) is less significant than the principal term N_i by the factor of the order of h/R. Neglecting this term in the principal terms in (28), we introduce the relative errors of the orders of Λ/R, h/R, $h^2/(\Lambda R)$, $h^3/(\Lambda^2 R)$, ... in the propagation velocity at each interface. The corresponding errors of the travel time are of the orders of $h\Lambda/(vR)$, $h^2/(vR)$, $h^3/(v\Lambda R)$, $h^4/(v\Lambda^2 R)$, ... at each interface. The corresponding relative error in terms of amplitude, caused by a single interface, are then of the orders of h/R, $h^2/(\Lambda R)$, $h^3/(\Lambda^2 R)$, $h^4/(\Lambda^3 R)$, ... that should be negligible for most of reasonably discretized models.

Errors of the same orders are also caused by neglecting term $\frac{1}{2}Z_{iJK}\xi_J\xi_K$ in (24) when substituting (24) into (25). The errors of the orders lower by the factors of h/Λ, $(h/\Lambda)^2$, $(h/\Lambda)^3$, and $(h/\Lambda)^4$ are caused if neglecting this term when substituting (24) into (28), (29), (31), and (33), respectively.

Finally, we may restrict (25), (28), (29), (31), and (33) in most cases to the following terms

(a) the wavefield

$$\begin{aligned} u_i(\xi_1,\xi_2) \approx & (U_i + U_{ij}Z_j + \frac{1}{2}U_{ijk}Z_jZ_k + \frac{1}{6}U_{ijkl}Z_jZ_kZ_l + \frac{1}{24}U_{ijklm}Z_jZ_kZ_lZ_m + ...) \\ & +(U_{ij}Z_{jJ} + U_{ijk}Z_{jJ}Z_k + \frac{1}{2}U_{ijkl}Z_{jJ}Z_kZ_l + \frac{1}{6}U_{ijklm}Z_{jJ}Z_kZ_lZ_m + ...)\xi_J \\ & +(\frac{1}{2}U_{ijk}Z_{jJ}Z_{kK} + \frac{1}{2}U_{ijkl}Z_{jJ}Z_{kK}Z_l + \frac{1}{4}U_{ijklm}Z_{jJ}Z_{kK}Z_lZ_m + ...)\xi_J\xi_K \\ & +(\frac{1}{6}U_{ijkl}Z_{jJ}Z_{kK}Z_{lL} + \frac{1}{6}U_{ijklm}Z_{jJ}Z_{kK}Z_{lL}Z_m + ...)\xi_J\xi_K\xi_L \\ & +(\frac{1}{24}U_{ijklm}Z_{jJ}Z_{kK}Z_{lL}Z_{mM} + ...)\xi_J\xi_K\xi_L\xi_M + ... \quad ; \end{aligned} \quad (34)$$

(b) the traction

$$
\begin{aligned}
[\sigma_{ij}n_j](\xi_1,\xi_2) \approx C_{ijkl}N_j[&(U_{kl} + U_{klm}Z_m + \frac{1}{2}U_{klmn}Z_mZ_n + \frac{1}{6}U_{klmnp}Z_mZ_nZ_p + ...) \\
&+(U_{klm}Z_{mJ} + U_{klmn}Z_{mJ}Z_n + \frac{1}{2}U_{klmnp}Z_{mJ}Z_nZ_p + ...)\xi_J \\
&+(\frac{1}{2}U_{klmn}Z_{mJ}Z_{nK} + \frac{1}{2}U_{klmnp}Z_{mJ}Z_{nK}Z_p + ...)\xi_J\xi_K \\
&+(\frac{1}{6}U_{klmnp}Z_{mJ}Z_{nK}Z_{pL} + ...)\xi_J\xi_K\xi_L + ...] \quad ; \qquad (35)
\end{aligned}
$$

(c) the second derivative of the wavefield with respect to time

$$
\begin{aligned}
u_{i,tt}(\xi_1,\xi_2) \approx \varrho^{-1}C_{ijkl}[&(U_{klj} + U_{kljm}Z_m + \frac{1}{2}U_{kljmn}Z_mZ_n + ...) \\
&+(U_{kljm}Z_{mJ} + U_{kljmn}Z_{mJ}Z_n + ...)\xi_J \\
&+(\frac{1}{2}U_{kljmn}Z_{mJ}Z_{nK} + ...)\xi_J\xi_K + ...] \quad ; \qquad (36)
\end{aligned}
$$

(d) the second derivative of the traction with respect to time

$$
\begin{aligned}
[\sigma_{ij,tt}n_j](\xi_1,\xi_2) \approx \varrho^{-1}C_{ijkl}N_jC_{kmnp}[&(U_{npml} + U_{npmlq}Z_q + \frac{1}{2}U_{npmlqr}Z_qZ_r + ...) \\
&(U_{npmlq}Z_{qJ} + U_{npmlqr}Z_{qJ}Z_r + ...)\xi_J \\
&(\frac{1}{2}U_{npmlqr}Z_{qJ}Z_{rK} + ...)\xi_J\xi_K + ...] \quad ; \qquad (37)
\end{aligned}
$$

(e) the fourth derivative of the wavefield with respect to time

$$
\begin{aligned}
u_{i,tttt}(\xi_1,\xi_2) \approx \varrho^{-2}C_{ijkl}C_{kmnp}[&(U_{npmlj} + U_{npmljq}Z_q + ...) \\
&(U_{npmljq}Z_{qJ} + ...)\xi_J + ...] \quad ; \qquad (38)
\end{aligned}
$$

(...) etc.

We arrange the coefficients of the Taylor expansions

$$
\begin{aligned}
u_n(\xi_1,\xi_2) &= m_n + m_{nJ}\xi_J + \frac{1}{2}m_{nJK}\xi_J\xi_K + \frac{1}{6}m_{nJKL}\xi_J\xi_K\xi_L \\
&\qquad + \frac{1}{24}m_{nJKLM}\xi_J\xi_K\xi_L\xi_M + ... \\
[\sigma_{ij}n_j](\xi_1,\xi_2) &= m_{n3} + m_{nJ3}\xi_J + \frac{1}{2}m_{nJK3}\xi_J\xi_K + \frac{1}{6}m_{nJKL3}\xi_J\xi_K\xi_L \\
&\qquad + \frac{1}{24}m_{nJKLM3}\xi_J\xi_K\xi_L\xi_M + ... \\
u_{n,tt}(\xi_1,\xi_2) &= m_{n33} + m_{nJ33}\xi_J + \frac{1}{2}m_{nJK33}\xi_J\xi_K + \frac{1}{6}m_{nJKL33}\xi_J\xi_K\xi_L + ... \\
[\sigma_{ij,tt}n_j](\xi_1,\xi_2) &= m_{n333} + m_{nJ333}\xi_J + \frac{1}{2}m_{nJK333}\xi_J\xi_K + ... \\
u_{n,tttt}(\xi_1,\xi_2) &= m_{n3333} + m_{nJ3333}\xi_J + ... \\
[\sigma_{ij,tttt}n_j](\xi_1,\xi_2) &= m_{n33333} + ... \quad , \qquad (39)
\end{aligned}
$$

of above quantities (a), (b), (c), (d), (e), ..., along the interface, into vector $\mathbf{m}$.

Then the quantities (a), (b), (c), (d), (e), ... at both sides of the structural interface are equal if and only if the vectors

$$\mathbf{m} = \mathbf{M}\mathbf{U} \tag{40}$$

at both sides of the interface are equal. Here $\mathbf{M}$ is the matrix projecting vector $\mathbf{U}$ of the wavefield derivatives onto the Taylor expansion coefficients $\mathbf{m}$ of the (a) wavefield, (b) traction, (c) second time derivatives of the wavefield, (d) second time derivatives of the traction, (e) fourth time derivatives of the wavefield, etc., along the interface.

Matrix elements, corresponding to approximations (34), (35), (36), (37), and (38), are

$$\mathbf{M} = \begin{pmatrix}
M_{n:i} & M_{n:ij} & M_{n:i[jk]} & M_{n:i[jkl]} & M_{n:i[jklm]} & \cdots \\
M_{n\,J:i} & M_{n\,J:ij} & M_{n\,J:i[jk]} & M_{n\,J:i[jkl]} & M_{n\,J:i[jklm]} & \cdots \\
M_{n\,JK:i} & M_{n\,JK:ij} & M_{n\,JK:i[jk]} & M_{n\,JK:i[jkl]} & M_{n\,JK:i[jklm]} & \cdots \\
M_{n\,JKL:i} & M_{n\,JKL:ij} & M_{n\,JKL:i[jk]} & M_{n\,JKL:i[jkl]} & M_{n\,JKL:i[jklm]} & \cdots \\
M_{n\,JKLM:i} & M_{n\,JKLM:ij} & M_{n\,JKLM:i[jk]} & M_{n\,JKLM:i[jkl]} & M_{n\,JKLM:i[jklm]} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
M_{n3:i} & M_{n3:ij} & M_{n3:i[jk]} & M_{n3:i[jkl]} & M_{n3:i[jklm]} & \cdots \\
M_{n\,J3:i} & M_{n\,J3:ij} & M_{n\,J3:i[jk]} & M_{n\,J3:i[jkl]} & M_{n\,J3:i[jklm]} & \cdots \\
M_{n\,JK3:i} & M_{n\,JK3:ij} & M_{n\,JK3:i[jk]} & M_{n\,JK3:i[jkl]} & M_{n\,JK3:i[jklm]} & \cdots \\
M_{n\,JKL3:i} & M_{n\,JKL3:ij} & M_{n\,JKL3:i[jk]} & M_{n\,JKL3:i[jkl]} & M_{n\,JKL3:i[jklm]} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
M_{n33:i} & M_{n33:ij} & M_{n33:i[jk]} & M_{n33:i[jkl]} & M_{n33:i[jklm]} & \cdots \\
M_{n\,J33:i} & M_{n\,J33:ij} & M_{n\,J33:i[jk]} & M_{n\,J33:i[jkl]} & M_{n\,J33:i[jklm]} & \cdots \\
M_{n\,JK33:i} & M_{n\,JK33:ij} & M_{n\,JK33:i[jk]} & M_{n\,JK33:i[jkl]} & M_{n\,JK33:i[jklm]} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
M_{n333:i} & M_{n333:ij} & M_{n333:i[jk]} & M_{n333:i[jkl]} & M_{n333:i[jklm]} & \cdots \\
M_{n\,J333:i} & M_{n\,J333:ij} & M_{n\,J333:i[jk]} & M_{n\,J333:i[jkl]} & M_{n\,J333:i[jklm]} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
M_{n3333:i} & M_{n3333:ij} & M_{n3333:i[jk]} & M_{n3333:i[jkl]} & M_{n3333:i[jklm]} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}$$

$$
= \begin{pmatrix}
\delta_{ni} & \delta_{ni}Z_j & \delta_{ni}Z_jZ_k & \delta_{ni}Z_jZ_kZ_l & \delta_{ni}Z_jZ_kZ_lZ_m & \cdots \\
0 & \delta_{ni}Z_{jJ} & 2\delta_{ni}Z_{\bar{j}J}Z_{\bar{k}} & 3\delta_{ni}Z_{\bar{j}J}Z_{\bar{k}}Z_{\bar{l}} & 4\delta_{ni}Z_{\bar{j}J}Z_{\bar{k}}Z_{\bar{l}}Z_{\bar{m}} & \cdots \\
0 & 0 & \delta_{ni}Z_{\bar{j}J}Z_{\bar{k}K} & 3\delta_{ni}Z_{\bar{j}J}Z_{\bar{k}K}Z_{\bar{l}} & 6\delta_{ni}Z_{\bar{j}J}Z_{\bar{k}K}Z_{\bar{l}}Z_{\bar{m}} & \cdots \\
0 & 0 & 0 & \delta_{ni}Z_{\bar{j}J}Z_{\bar{k}K}Z_{\bar{l}L} & 4\delta_{ni}Z_{\bar{j}J}Z_{\bar{k}K}Z_{\bar{l}L}Z_{\bar{m}} & \cdots \\
0 & 0 & 0 & 0 & \delta_{ni}Z_{\bar{j}J}Z_{\bar{k}K}Z_{\bar{l}L}Z_{\bar{m}M} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
0 & C_{ijns}N_s & C_{i\bar{j}ns}N_sZ_{\bar{k}} & C_{i\bar{j}ns}N_sZ_{\bar{k}}Z_{\bar{l}} & C_{i\bar{j}ns}N_sZ_{\bar{k}}Z_{\bar{l}}Z_{\bar{m}} & \cdots \\
0 & 0 & C_{i\bar{j}ns}N_sZ_{\bar{k}J} & 2C_{i\bar{j}ns}N_sZ_{\bar{k}J}Z_{\bar{l}} & 3C_{i\bar{j}ns}N_sZ_{\bar{k}J}Z_{\bar{l}}Z_{\bar{m}} & \cdots \\
0 & 0 & 0 & C_{i\bar{j}ns}N_sZ_{\bar{k}J}Z_{\bar{l}K} & 3C_{i\bar{j}ns}N_sZ_{\bar{k}J}Z_{\bar{l}K}Z_{\bar{m}} & \cdots \\
0 & 0 & 0 & 0 & C_{ijns}N_sZ_{kJ}Z_{lK}Z_{mL} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & \varrho^{-1}C_{i\bar{j}\bar{k}n} & \varrho^{-1}C_{i\bar{j}\bar{k}n}Z_{\bar{l}} & \varrho^{-1}C_{i\bar{j}\bar{k}n}Z_{\bar{l}}Z_{\bar{m}} & \cdots \\
0 & 0 & 0 & \varrho^{-1}C_{i\bar{j}\bar{k}n}Z_{\bar{l}J} & 2\varrho^{-1}C_{i\bar{j}\bar{k}n}Z_{\bar{l}J}Z_{\bar{m}} & \cdots \\
0 & 0 & 0 & 0 & \varrho^{-1}C_{i\bar{j}\bar{k}n}Z_{\bar{l}J}Z_{\bar{m}K} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & 0 & \varrho^{-1}C_{i\bar{j}\bar{k}r}C_{r\bar{l}ns}N_s & \varrho^{-1}C_{i\bar{j}\bar{k}r}C_{r\bar{l}ns}N_sZ_{\bar{m}} & \cdots \\
0 & 0 & 0 & 0 & \varrho^{-1}C_{i\bar{j}\bar{k}r}C_{r\bar{l}ns}N_sZ_{\bar{m}J} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & 0 & 0 & \varrho^{-2}C_{i\bar{j}\bar{k}r}C_{r\bar{l}\bar{m}n} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix} . \qquad (41)
$$

The expressions for the matrix elements on the right–hand side of (41) have to be averaged over all permutations of indices j, k, l, m. For convenience, these indices are marked by bars: $\bar{j}, \bar{k}, \bar{l}, \bar{m}$.

Let us denote the geological block containing central point $\mathbf{x}$ by index $\alpha = 0$, and other M geological blocks containing the points influencing the finite–difference scheme at $\mathbf{x}$ by indices $\alpha = 1, 2, ..., M$. Most frequently, there will be just a single interface in the vicinity of $\mathbf{x}$: $M = 1$. We denote by $\mathbf{U}^\alpha$, $\alpha = 0, 1, ..., M$ the vectors of partial derivatives of the wavefield in the α^{th} geological block, and by $\mathbf{M}^{\beta\alpha}$, $\beta = 0, 1, ..., M$, $\alpha = 0, 1, ..., M$ matrix (41) corresponding to the expansion of the wavefield in the α^{th} geological block along the interface between the α^{th} and β^{th} blocks. The matching of the wavefields between the α^{th} block and β^{th} block may now be expressed by means of equation

$$
\mathbf{M}^{\beta\alpha}\mathbf{U}^\alpha = \mathbf{M}^{\alpha\beta}\mathbf{U}^\beta \quad , \qquad (42)
$$

where no summation is performed over α and β.

It is clear from the structure of matrix (41) that a component of vector $\mathbf{U}$ has no influence onto the components of $\mathbf{m}$ with more indices. Similarly, if inverting equation (40), a component of vector $\mathbf{m}$ has no influence onto the components of $\mathbf{U}$ with more indices. It is thus sufficient to consider in each geological block α only the components of $\mathbf{U}^\alpha$ and $\mathbf{m}^\alpha$ with the number of indices not exceeding the maximum number of indices of $\mathbf{U}^0$, considered at central point $\mathbf{x}$, and, of course, only the corresponding elements of matrix $\mathbf{M}$. Matrix $\mathbf{M}$ may then be inverted by parts, according to the number of indices of its elements.

5 Finite–difference schemes at structural interfaces

From the wavefield matching equations (42), we select M equations matching the wavefields in the 0^{th} block with the wavefields in the other M blocks,

$$\mathbf{M}^{\alpha 0}\mathbf{U}^{0} = \mathbf{M}^{0\alpha}\mathbf{U}^{\alpha}, \ \alpha = 1, 2, ..., M \quad , \tag{43}$$

where no summation is performed over α. We do not attempt to mutually match the wavefields between the 1^{st} and 2^{nd} block, 1^{st} and 3^{rd} block, 2^{nd} and 3^{rd} block, etc., if there are more than one structural interfaces in the vicinity of central point $\mathbf{x}$.

Let us introduce simple filtering (projection) matrices $\mathbf{P}^{\alpha}$, filtering the gridpoint values according to geological blocks $\alpha = 0, 1, ..., M$. If a wavefield value is taken at the gridpoint situated in the α^{th} geological block, the corresponding diagonal element of $\mathbf{P}^{\alpha}$ is 1. All other elements are 0. Thus

$$\sum_{\alpha=0}^{M} \mathbf{P}^{\alpha} = \mathbf{1} \quad , \tag{44}$$

where $\mathbf{1}$ is an identity matrix. The Taylor expansion of the wavefield may then be expressed in the form of

$$\mathbf{u} = \sum_{\alpha=0}^{M} \mathbf{P}^{\alpha}\mathbf{T}\mathbf{U}^{\alpha} \quad , \tag{45}$$

which is a generalization of equation (6) at structural interfaces. If there were no interfaces in the vicinity of $\mathbf{x}$, $M = 0$, $\mathbf{P}^{0}$ would be an identity matrix and (45) would coincide with (6).

Substituting (43) into (45), we may express wavefield values $\mathbf{u}$ in terms of $\mathbf{U}^{0}$,

$$\mathbf{u} = \sum_{\alpha=0}^{M} \mathbf{P}^{\alpha}\mathbf{T}(\mathbf{M}^{0\alpha})^{-1}\mathbf{M}^{\alpha 0}\mathbf{U}^{0} \quad . \tag{46}$$

Then

$$\mathbf{U}^{0} = \left[\sum_{\alpha=0}^{M} \mathbf{P}^{\alpha}\mathbf{T}(\mathbf{M}^{0\alpha})^{-1}\mathbf{M}^{\alpha 0}\right]^{-1}\mathbf{u} = \left[\mathbf{P}^{0}\mathbf{T} + \sum_{\alpha=1}^{M} \mathbf{P}^{\alpha}\mathbf{T}(\mathbf{M}^{0\alpha})^{-1}\mathbf{M}^{\alpha 0}\right]^{-1}\mathbf{u} \tag{47}$$

may be substituted into (18) to arrive at the final matrix form of the finite–difference scheme in the vicinity of structural interfaces,

$$\mathbf{t} = \mathbf{S}\left[\mathbf{P}^{0}\mathbf{T} + \sum_{\alpha=1}^{M} \mathbf{P}^{\alpha}\mathbf{T}(\mathbf{M}^{0\alpha})^{-1}\mathbf{M}^{\alpha 0}\right]^{-1}\mathbf{u} \quad . \tag{48}$$

6 Free space

The wavefield (in terms of displacement) in a free space (vacuum) should be calculated in the same way as in the material geological blocks. The density in a free space is zero, $\varrho = 0$. On the other hand, the reduced elastic parameters $\varrho^{-1}c_{ijkl}$, corresponding to the squares of propagation velocities, should be chosen reasonably, especially with regard to the grid step.

For instance, to analytically continue the reduced elastic parameters $\varrho^{-1}c_{ijkl}$ from the neighbouring geological block to the free space, seems to be a very good choice. Then some rows in matrix (41), corresponding to free space, are identical with those corresponding to the neighbouring geological block, whereas other rows are annulled.