

# An integral equation approach using a CG-FFT technique for 3-D elastic wave modelling

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## Abstract

In this paper, we solve a forward scattering problem for three-dimensional full-space elastic wave modelling. A system of integral equations in terms of the stress tensor and the particle velocities, instead of the displacements, is formulated. By using this new system of integral equations, we have no differentiations inside the integrals, which reduces the complexity of the numerical implementation. A CG-FFT technique is applied to solve the discretized linear system. Moreover, several pre-conditioners and approximations have been implemented, which are shown to increase the computational efficiency in the numerical tests.

*Key words:* Elastic, 3-D, CG-FFT, Integral Equation

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## 1 Introduction

The study of elastic wave propagation plays an important role in geophysical prospecting, non-destructive testing and biomedical applications. One of the most essential problems in this field is 3-D full-space scattering from inhomogeneous elastic inclusions excited by a given time-harmonic source. Since this problem is considered as the basis to the inverse problem, it has to be solved effectively and efficiently. A lot of investigations have been taken to solve this problem, such as Guzina and co-authors [17,18], Liu and Rizzo [19,20], Habashy and co-authors [9,10,8]. These authors solve for the displacements directly in their work.

In this paper, we choose to first solve a formulation of elastodynamic governing equations regarding the stress tensor and the particle velocities [1], then obtain the displacements from the particle velocities. In this way, the system of partial differential equations is of first-order, therefore, has less differential operators than the one having the displacements as the unknown variables, which is of second-order.

Unlike in [17–20], we handle the problem by employing a volume integral equation approach, where the computational domain could be restricted, hence, the number of unknowns will be reduced. Note that the choice of the computational domain depends only on the distribution of the inhomogeneities, regardless of the locations of the sources and receivers.

Furthermore, this new system of integral equations has no differential operators inside the integrals. In other words, no differentiations are working directly on the fields. Therefore, only the derivatives of the Green’s functions need to be taken care of, which can be handled by finite difference schemes.

Due to the singularity of the Green’s functions, we take a weakening procedure before we compute the integrals numerically, where the spherical means of the vector potentials are used instead of their point values. This allows us to obtain the vector potentials efficiently and accurately. Taking advantage of the translational invariance of the Helmholtz Green’s functions, we are able to calculate the convolutions efficiently by using FFT routines [6]. Taking into account of the huge amount of the unknowns and highly full size of the matrix, the conjugate gradient methods such as CGNR [3] and BiCGStab [15] are employed to solve the discretized linear system.

In addition to attacking the system of integral equations by means of the linear equations solvers, we approximate it by applying the so-called EBA (Extended Born Approximation) technique [7]. This technique is also applied to a variation of the interested system of integral equations. It is shown that these approximations work better than the conventional Born approximation [21,11], and their performances are improving when we decrease the frequency of operation.

Moreover, to accelerate the convergence rate of the iterative linear equation solvers, two sorts of pre-conditioners are investigated. One is simply a diagonal matrix, which is extracted from the matrix of the linear system. Another is the EBA of the integral equations [4]. Both of them have helped to improve the condition of the matrix, when the latter appears to be better.

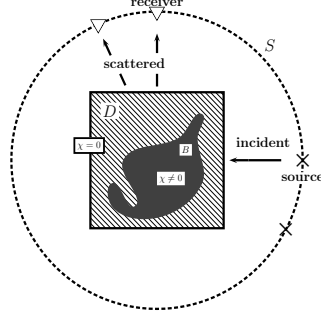


Fig. 1. The scattering experiment configuration.

## 2 Scattering problem and governing equations

In an isotropic, linear and instantaneously reacting solid, we consider a scattering problem of an inhomogeneous object occupying the domain  $D$  in a homogeneous background. The scatterer  $B$  is elastodynamically irradiated by given sources located in the embedding, see Figure 1. The problem is to determine the total elastic wavefield in the given configuration.

Following the elastic wave theory and the notations in [1], the elastic wave motion in the frequency domain with time factor  $\exp(st)$  is written as

$$-\Delta_{k,m,p,q} \partial_m \tau_{p,q} + s \rho v_k = f_k, \quad (1)$$

$$\Delta_{i,j,m,r} \partial_m v_r - s S_{i,j,p,q} \tau_{p,q} = h_{i,j}, \quad (2)$$

where  $\partial_m$  is the partial differential operator,  $\tau_{p,q}$  is the stress tensor,  $v_k$  is the particle velocity,  $\rho$  is the mass density and  $S_{i,j,p,q}$  is the compliance tensor written as

$$S_{i,j,p,q} = 3\Lambda \Delta_{i,j,p,q}^\delta + 2M \Delta_{i,j,p,q}, \quad (3)$$

in which  $\Delta_{i,j,p,q}^\delta$  and  $\Delta_{i,j,p,q}$  are unit tensors of rank four and defined as

$$\Delta_{i,j,p,q}^\delta = \frac{1}{3} \delta_{i,j} \delta_{p,q}, \quad (4)$$

$$\Delta_{i,j,p,q} = \frac{1}{2} (\delta_{i,p} \delta_{j,q} + \delta_{i,q} \delta_{j,p}). \quad (5)$$

On the right hand side of the above governing equations,  $f_k$  is the force source

and  $h_{i,j}$  is the deformation rate source. All the subscripts could be taken on value of 1, 2 or 3, and they follow the so-called ‘‘summation convention’’ rule.

Note that those unit tensors have the following properties:

$$\Delta_{i,j,p,q}^{\delta} \Delta_{p,q,k,l}^{\delta} = \Delta_{i,j,k,l}^{\delta}, \quad (6)$$

$$\Delta_{i,j,p,q}^{\delta} \Delta_{p,q,k,l}^{\delta} = \Delta_{i,j,k,l}^{\delta}, \quad (7)$$

$$\Delta_{i,j,p,q}^{\delta} \Delta_{p,q,k,l}^{\delta} = \Delta_{i,j,k,l}^{\delta}. \quad (8)$$

These unit tensors are linear independent, while for contracted subscripts we note that  $\Delta_{i,j,p,p}^{\delta} = \Delta_{i,j,p,p}^{\delta} = \delta_{i,j}$ , where  $\delta_{i,j}$  is Kronecker’s unit tensor of rank two. The parameters  $\Lambda$  and  $M$  are related to the Lamé coefficients  $\lambda$  and  $\mu$  as follows:

$$\lambda = \frac{-\Lambda}{2M(3\Lambda + 2M)}, \quad \mu = \frac{1}{4M}, \quad (9)$$

$$\Lambda = \frac{-\lambda}{2\mu(3\lambda + 2\mu)}, \quad M = \frac{1}{4\mu}. \quad (10)$$

Moreover, in this study, we choose to work with the particle velocity vector  $v_r$  instead of the displacement vector  $U_r$ . The relation between these two vectors are given by,

$$v_r = s U_r. \quad (11)$$

In the scattering problem, the elastodynamic properties of the embedding are characterized by the material quantities  $\rho$ ,  $\Lambda$  and  $M$ , and the elastodynamic properties of the scatterer are characterized by the material quantities  $\rho^{\text{sct}}(\mathbf{x})$ ,  $\Lambda^{\text{sct}}(\mathbf{x})$  and  $M^{\text{sct}}(\mathbf{x})$ , where  $\mathbf{x}$  is the three-dimensional (3D) spatial position vector. Therefore, mathematically speaking, we are interested in solving Eq.(1) and Eq.(2) for wavefield  $\{\tau_{p,q}, v_r\}$  when the sources  $f_k$  and  $h_{i,j}$  and the material properties  $\rho$ ,  $\Lambda$ ,  $M$ ,  $\rho^{\text{sct}}(\mathbf{x})$ ,  $\Lambda^{\text{sct}}(\mathbf{x})$  and  $M^{\text{sct}}(\mathbf{x})$  are given.

### 3 Formulation of field integral equations

#### 3.1 Expressions of the incident wavefields

The standard procedure is to calculate first the so-called incident elastic wavefield,  $\{\tau_{p,q}^{\text{inc}}, v_r^{\text{inc}}\}$ , i.e. the wavefield that would be present in the configuration

if the object shows no contrast with respect to its embedding. Theoretically, the incident wavefield can be obtained through [1]:

$$-\tau_{p,q}^{\text{inc}}(\mathbf{x}) = \int [G_{p,q,i,j}^{\tau,h}(\mathbf{x}-\mathbf{x}')h_{i,j}(\mathbf{x}') + G_{p,q,k}^{\tau,f}(\mathbf{x}-\mathbf{x}')f_k(\mathbf{x}')]d\mathbf{x}', \quad (12)$$

$$v_r^{\text{inc}}(\mathbf{x}) = \int [G_{r,i,j}^{v,h}(\mathbf{x}-\mathbf{x}')h_{i,j}(\mathbf{x}') + G_{r,k}^{v,f}(\mathbf{x}-\mathbf{x}')f_k(\mathbf{x}')]d\mathbf{x}', \quad (13)$$

where  $G_{p,q,i,j}^{\tau,h}$  is the stress/deformation rate source Green's function,  $G_{p,q,k}^{\tau,f}$  is the stress/force source Green's function,  $G_{r,i,j}^{v,h}$  is the particle velocity/deformation rate source Green's function and  $G_{r,k}^{v,f}$  is the particle velocity/force source Green's function. More precisely,

$$G_{p,q,i,j}^{\tau,h}(\mathbf{x}) = -\frac{1}{s}C_{p,q,i,j}\delta(\mathbf{x}) - \frac{1}{s\rho}C_{p,q,n,r}C_{k,m,i,j}\partial_n\partial_m G_{r,k}(\mathbf{x}, s), \quad (14)$$

$$G_{p,q,k}^{\tau,f}(\mathbf{x}) = \frac{1}{\rho}C_{p,q,n,r}\partial_n G_{r,k}(\mathbf{x}), \quad (15)$$

$$G_{r,i,j}^{v,h}(\mathbf{x}) = -\frac{1}{\rho}C_{k,m,i,j}\partial_m G_{r,k}(\mathbf{x}), \quad (16)$$

$$G_{r,k}^{v,f}(\mathbf{x}) = \frac{s}{\rho}G_{r,k}(\mathbf{x}), \quad (17)$$

and

$$G_{r,k}(\mathbf{x}) = \frac{1}{c_s^2}\delta_{r,k}G_s(\mathbf{x}) + \frac{1}{s^2}\partial_r\partial_k(G_p - G_s)(\mathbf{x}), \quad (18)$$

in which

$$G_p(\mathbf{x}) = \frac{\exp(-\frac{s}{c_p}|\mathbf{x}|)}{4\pi|\mathbf{x}|} \quad \text{and} \quad G_s(\mathbf{x}) = \frac{\exp(-\frac{s}{c_s}|\mathbf{x}|)}{4\pi|\mathbf{x}|}, \quad (19)$$

are the Helmholtz green's functions. Here  $c_p = \sqrt{\frac{\lambda+2\mu}{\rho}}$  and  $c_s = \sqrt{\frac{\mu}{\rho}}$  are the compressional wave speed and the shear wave speed of the embedding respectively. Further,  $C_{i,j,p,q}$  is the stiffness tensor. In terms of the Lamé coefficients we have

$$C_{i,j,p,q} = 3\lambda\Delta_{i,j,p,q}^\delta + 2\mu\Delta_{i,j,p,q} = \lambda\delta_{i,j}\delta_{p,q} + \mu(\delta_{i,p}\delta_{j,q} + \delta_{i,q}\delta_{j,p}). \quad (20)$$

Especially, when we have a monochromatic point force source located at  $\mathbf{x}^s$  and oriented in  $\alpha$ -direction, i.e.,

$$f_k(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}^s)\delta_{k,\alpha}, \quad \text{and} \quad h_{i,j}(\mathbf{x}) = 0, \quad (21)$$

the incident wave fields are given by

$$-\tau_{p,q}^{\text{inc}}(\mathbf{x}) = \int G_{p,q,k}^{\tau,f}(\mathbf{x} - \mathbf{x}')\delta(\mathbf{x}' - \mathbf{x}^s)\delta_{k,\alpha}d\mathbf{x}' = G_{p,q,\alpha}^{\tau,f}(\mathbf{x} - \mathbf{x}^s), \quad (22)$$

$$v_r^{\text{inc}}(\mathbf{x}) = \int G_{r,k}^{v,f}(\mathbf{x} - \mathbf{x}')\delta(\mathbf{x}' - \mathbf{x}^s)\delta_{k,\alpha}d\mathbf{x}' = G_{r,\alpha}^{v,f}(\mathbf{x} - \mathbf{x}^s). \quad (23)$$

### 3.2 Expressions of the scattered wavefields

Next the scattered wavefield is obtained as follows:

$$\tau_{p,q}^{\text{sct}} = \tau_{p,q} - \tau_{p,q}^{\text{inc}}, \quad v_r^{\text{sct}} = v_r - v_r^{\text{inc}}, \quad (24)$$

and, through a particular reasoning, the problem of determining the scattered wavefield is reduced to calculating its equivalent contrast source distribution, whose common support will be the domain  $D$  occupied by the scatterer.

Since the contrasts in the medium properties vanish outside the scattering object, the scattered field can be written as follows:

$$-\tau_{p,q}^{\text{sct}}(\mathbf{x}) = \int_D [G_{p,q,i,j}^{\tau,h}(\mathbf{x} - \mathbf{x}')h_{i,j}^{\text{sct}}(\mathbf{x}') + G_{p,q,k}^{\tau,f}(\mathbf{x} - \mathbf{x}')f_k^{\text{sct}}(\mathbf{x}')]d\mathbf{x}', \quad (25)$$

$$v_r^{\text{sct}}(\mathbf{x}) = \int_D [G_{r,i,j}^{v,h}(\mathbf{x} - \mathbf{x}')h_{i,j}^{\text{sct}}(\mathbf{x}') + G_{r,k}^{v,f}(\mathbf{x} - \mathbf{x}')f_k^{\text{sct}}(\mathbf{x}')]d\mathbf{x}', \quad (26)$$

The contrast sources  $h_{i,j}^{\text{sct}}(\mathbf{x})$  and  $f_k^{\text{sct}}(\mathbf{x})$  may be expressed in terms of the total wavefields through

$$\begin{aligned} h_{i,j}^{\text{sct}}(\mathbf{x}) &= s[S_{i,j,p,q}^{\text{sct}}(\mathbf{x}) - S_{i,j,p,q}]\tau_{p,q}(\mathbf{x}) \\ &= s\Lambda\chi^\Lambda(\mathbf{x})\delta_{i,j}\tau_{k,k}(\mathbf{x}) + sM\chi^M(\mathbf{x})[\tau_{i,j}(\mathbf{x}) + \tau_{j,i}(\mathbf{x})], \end{aligned} \quad (27)$$

$$f_k^{\text{sct}}(\mathbf{x}) = -s\rho\chi^\rho(\mathbf{x})v_k(\mathbf{x}), \quad (28)$$

where the three contrast quantities  $\chi^\rho$ ,  $\chi^\Lambda$  and  $\chi^M$  are given by

$$\chi^\Lambda(\mathbf{x}) = \frac{\Lambda^{\text{sct}}(\mathbf{x})}{\Lambda} - 1, \quad \chi^M(\mathbf{x}) = \frac{M^{\text{sct}}(\mathbf{x})}{M} - 1, \quad \chi^\rho(\mathbf{x}) = \frac{\rho^{\text{sct}}(\mathbf{x})}{\rho} - 1. \quad (29)$$

We finally note that, once the contrast sources  $f_k^{\text{sct}}(\mathbf{x})$  and  $h_{i,j}^{\text{sct}}(\mathbf{x})$  are known, the scattered field may be calculated using the source type of integral representations of Eqs. (25) - (26).

### 3.3 Equations inside the computational domain

The total wavefield inside the object is determined from the Eqs. (25) - (26), by letting the point of observation to be inside the test domain  $D$ . We then obtain the system of integral equations

$$\begin{aligned} \tau_{p,q}^{\text{inc}}(\mathbf{x}) = & \tau_{p,q}(\mathbf{x}) + s \int_D \left[ G_{p,q,i,i}^{\tau,h}(\mathbf{x} - \mathbf{x}') \Lambda \chi^\Lambda(\mathbf{x}') \tau_{k,k}(\mathbf{x}') \right. \\ & \left. + G_{p,q,i,j}^{\tau,h}(\mathbf{x} - \mathbf{x}') 2M \chi^M(\mathbf{x}') \tau_{i,j}(\mathbf{x}') - G_{p,q,k}^{\tau,f}(\mathbf{x} - \mathbf{x}') \rho \chi^\rho(\mathbf{x}') v_k(\mathbf{x}') \right] d\mathbf{x}', \end{aligned} \quad (30)$$

$$\begin{aligned} v_r^{\text{inc}}(\mathbf{x}) = & v_r(\mathbf{x}) - s \int_D \left[ G_{r,i,i}^{v,h}(\mathbf{x} - \mathbf{x}') \Lambda \chi^\Lambda(\mathbf{x}') \tau_{k,k}(\mathbf{x}') \right. \\ & \left. + G_{r,i,j}^{v,h}(\mathbf{x} - \mathbf{x}') 2M \chi^M(\mathbf{x}') \tau_{i,j}(\mathbf{x}') - G_{r,k}^{v,f}(\mathbf{x} - \mathbf{x}') \rho \chi^\rho(\mathbf{x}') v_k(\mathbf{x}') \right] d\mathbf{x}', \end{aligned} \quad (31)$$

for  $\mathbf{x} \in D$ . This is a system of integral equations for the six unknown components of the symmetric stress tensor  $\tau_{p,q}$  and the three components of the particle velocity vector  $v_r$ .

### 3.4 Normalized field integral equations

Since the ratio of the magnitude of the stress tensor and the magnitude of the particle velocity vector is so big that it will make the linear system ill-conditioned, we take as the normalization constant the S-wave impedance as  $Z_s = \rho c_s$  and we propose to work with the re-normalized equations.

Define  $u_r = Z_s v_r$ . After a few manipulations, the re-normalized equations of wavefield  $\{\tau_{p,q}, u_r\}$  are obtained as follows:

$$\begin{aligned}
\tau_{p,q}^{\text{inc}}(\mathbf{x}) &= \tau_{p,q}(\mathbf{x}) + s\Lambda \int_D G_{p,q,i,i}^{\tau,h}(\mathbf{x}-\mathbf{x}')\chi^\Lambda(\mathbf{x}')\tau_{k,k}(\mathbf{x}')d\mathbf{x}' \\
&\quad + 2sM \int_D G_{p,q,i,j}^{\tau,h}(\mathbf{x}-\mathbf{x}')\chi^M(\mathbf{x}')\tau_{i,j}(\mathbf{x}')d\mathbf{x}' - \frac{s}{c_s} \int_D G_{p,q,k}^{\tau,f}(\mathbf{x}-\mathbf{x}')\chi^\rho(\mathbf{x}')u_k(\mathbf{x}')d\mathbf{x}' \\
&= \tau_{p,q}(\mathbf{x}) + B_{p,q}^{\tau,\Lambda}(\mathbf{x}) + B_{p,q}^{\tau,M}(\mathbf{x}) + B_{p,q}^{\tau,\rho}(\mathbf{x}), \tag{32}
\end{aligned}$$

$$\begin{aligned}
\rho c_s v_r^{\text{inc}}(\mathbf{x}) &= u_r(\mathbf{x}) - \rho c_s s\Lambda \int_D G_{r,i,i}^{v,h}(\mathbf{x}-\mathbf{x}')\chi^\Lambda(\mathbf{x}')\tau_{k,k}(\mathbf{x}')d\mathbf{x}' \\
&\quad - 2\rho c_s sM \int_D G_{r,i,j}^{v,h}(\mathbf{x}-\mathbf{x}')\chi^M(\mathbf{x}')\tau_{i,j}(\mathbf{x}')d\mathbf{x}' + s\rho \int_D G_{r,k}^{v,f}(\mathbf{x}-\mathbf{x}')\chi^\rho(\mathbf{x}')u_k(\mathbf{x}')d\mathbf{x}' \\
&= u_r(\mathbf{x}) + B_r^{u,\Lambda}(\mathbf{x}) + B_r^{u,M}(\mathbf{x}) + B_r^{u,\rho}(\mathbf{x}), \tag{33}
\end{aligned}$$

where

$$B_{p,q}^{\tau,\Lambda}(\mathbf{x}) = \frac{\lambda}{2\mu} \left\{ \delta_{p,q} \left[ \frac{2c_s^2}{c_p^2} \chi^\Lambda(\mathbf{x})\tau_{k,k}(\mathbf{x}) + \frac{\lambda s^2}{\rho c_p^4} A^{p,\Lambda}(\mathbf{x}) \right] + \frac{2c_s^2}{c_p^2} \partial_p \partial_q A^{p,\Lambda}(\mathbf{x}) \right\}, \tag{34}$$

$$\begin{aligned}
B_{p,q}^{\tau,M}(\mathbf{x}) &= -\frac{\lambda}{2\mu} \left\{ \delta_{p,q} \left[ \frac{2c_s^2}{c_p^2} \chi^M(\mathbf{x})\tau_{k,k}(\mathbf{x}) + \frac{\lambda s^2}{\rho c_p^4} A^{p,M}(\mathbf{x}) + \frac{2c_s^2}{c_p^2} \partial_i \partial_j A_{i,j}^{p,M}(\mathbf{x}) \right] \right. \\
&\quad \left. + \frac{2c_s^2}{c_p^2} \partial_p \partial_q A^{p,M}(\mathbf{x}) \right\} - \chi^M(\mathbf{x})\tau_{p,q}(\mathbf{x}) - \left[ \partial_p \partial_j A_{j,q}^{s,M}(\mathbf{x}) + \partial_q \partial_j A_{j,p}^{s,M}(\mathbf{x}) \right] \\
&\quad - \frac{2c_s^2}{s^2} \partial_p \partial_q \partial_i \partial_j \left( A_{i,j}^{p,M} - A_{i,j}^{s,M} \right)(\mathbf{x}), \tag{35}
\end{aligned}$$

$$B_{p,q}^{\tau,\rho}(\mathbf{x}) = -\frac{\lambda}{\rho c_p^2} \frac{s}{c_s} \delta_{p,q} \partial_k A_k^{p,\rho}(\mathbf{x}) - \frac{s}{c_s} \left[ \partial_p A_q^{s,\rho}(\mathbf{x}) + \partial_q A_p^{s,\rho}(\mathbf{x}) \right] - \frac{2\mu}{s\rho c_s} \partial_p \partial_q \partial_k \left( A_k^{p,\rho} - A_k^{s,\rho} \right)(\mathbf{x}), \tag{36}$$

$$B_r^{u,\Lambda}(\mathbf{x}) = -\frac{\lambda s c_s}{2\mu c_p^2} \partial_r A^{p,\Lambda}(\mathbf{x}), \tag{37}$$

$$B_r^{u,M}(\mathbf{x}) = \frac{\lambda s c_s}{2\mu c_p^2} \partial_r A^{p,M}(\mathbf{x}) + \frac{s\rho c_s}{\mu} \partial_i A_{r,i}^{s,M}(\mathbf{x}) + \frac{c_s}{s} \partial_r \partial_i \partial_j \left( A_{i,j}^{p,M} - A_{i,j}^{s,M} \right)(\mathbf{x}), \tag{38}$$

and

$$B_r^{u,\rho}(\mathbf{x}) = \frac{s^2}{c_s^2} A_r^{s,\rho}(\mathbf{x}) + \partial_r \partial_k \left( A_k^{p,\rho} - A_k^{s,\rho} \right)(\mathbf{x}). \tag{39}$$

Here, the vector potentials are given by

$$A_{i,j}^{\gamma,\beta}(\mathbf{x}) = \int_D G_\gamma(\mathbf{x}-\mathbf{x}') \chi^\beta(\mathbf{x}') \tau_{k,k}(\mathbf{x}') d\mathbf{x}', \quad (40)$$

$$A_r^{\gamma,\rho}(\mathbf{x}) = \int_D G_\gamma(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') u_r(\mathbf{x}') d\mathbf{x}', \quad (41)$$

and  $A_{k,k}^{\gamma,\beta}(\mathbf{x})$  is abbreviated by  $A^{\gamma,\beta}(\mathbf{x})$ , where  $\gamma \in \{p, s\}$  and  $\beta \in \{\Lambda, M\}$ .

### 3.5 Normalized field integral equations of the scattered wavefields

One variation of Eq.(32) and Eq.(33) is to split the total fields on the right-hand side into two parts: incident fields and scattered fields, i.e.,

$$\begin{aligned} \tau_{p,q}^{\text{inc}}(\mathbf{x}) &= \tau_{p,q}^{\text{inc}}(\mathbf{x}) + \tau_{p,q}^{\text{sct}}(\mathbf{x}) + s\Lambda \int_D G_{p,q,i,i}^{\tau,h}(\mathbf{x}-\mathbf{x}') \chi^\Lambda(\mathbf{x}') [\tau_{k,k}^{\text{inc}}(\mathbf{x}') + \tau_{k,k}^{\text{sct}}(\mathbf{x}')] d\mathbf{x}' \\ &\quad + 2sM \int_D G_{p,q,i,j}^{\tau,h}(\mathbf{x}-\mathbf{x}') \chi^M(\mathbf{x}') [\tau_{i,j}^{\text{inc}}(\mathbf{x}') + \tau_{i,j}^{\text{sct}}(\mathbf{x}')] d\mathbf{x}' \\ &\quad - \frac{s}{c_s} \int_D G_{p,q,k}^{\tau,f}(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') [u_k^{\text{inc}}(\mathbf{x}') + u_k^{\text{sct}}(\mathbf{x}')] d\mathbf{x}', \end{aligned} \quad (42)$$

$$\begin{aligned} u_r^{\text{inc}}(\mathbf{x}) &= u_r^{\text{inc}}(\mathbf{x}) + u_r^{\text{sct}}(\mathbf{x}) - \rho c_s s \Lambda \int_D G_{r,i,i}^{v,h}(\mathbf{x}-\mathbf{x}') \chi^\Lambda(\mathbf{x}') [\tau_{k,k}^{\text{inc}}(\mathbf{x}') + \tau_{k,k}^{\text{sct}}(\mathbf{x}')] d\mathbf{x}' \\ &\quad - 2\rho c_s s M \int_D G_{r,i,j}^{v,h}(\mathbf{x}-\mathbf{x}') \chi^M(\mathbf{x}') [\tau_{i,j}^{\text{inc}}(\mathbf{x}') + \tau_{i,j}^{\text{sct}}(\mathbf{x}')] d\mathbf{x}' \\ &\quad + s\rho \int_D G_{r,k}^{v,f}(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') [u_k^{\text{inc}}(\mathbf{x}') + u_k^{\text{sct}}(\mathbf{x}')] d\mathbf{x}'. \end{aligned} \quad (43)$$

After moving every terms that involve the incident wavefields to the left-hand-side, we get

$$\begin{aligned} \tau_{p,q}^{\text{new}}(\mathbf{x}) &= \tau_{p,q}^{\text{sct}}(\mathbf{x}) + s\Lambda \int_D G_{p,q,i,i}^{\tau,h}(\mathbf{x}-\mathbf{x}') \chi^\Lambda(\mathbf{x}') \tau_{k,k}^{\text{sct}}(\mathbf{x}') d\mathbf{x}' \\ &\quad + 2sM \int_D G_{p,q,i,j}^{\tau,h}(\mathbf{x}-\mathbf{x}') \chi^M(\mathbf{x}') \tau_{i,j}^{\text{sct}}(\mathbf{x}') d\mathbf{x}' \end{aligned}$$

$$-\frac{s}{c_s} \int_D G_{p,q,k}^{\tau,f}(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') u_k^{\text{sct}}(\mathbf{x}') d\mathbf{x}', \quad (44)$$

$$\begin{aligned} u_r^{\text{new}}(\mathbf{x}) &= u_r^{\text{sct}}(\mathbf{x}) - \rho c_s s \Lambda \int_D G_{r,i,i}^{v,h}(\mathbf{x}-\mathbf{x}') \chi^\Lambda(\mathbf{x}') \tau_{k,k}^{\text{sct}}(\mathbf{x}') d\mathbf{x}' \\ &\quad - 2\rho c_s s M \int_D G_{r,i,j}^{v,h}(\mathbf{x}-\mathbf{x}') \chi^M(\mathbf{x}') \tau_{i,j}^{\text{sct}}(\mathbf{x}') d\mathbf{x}' \\ &\quad + s\rho \int_D G_{r,k}^{v,f}(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') u_k^{\text{sct}}(\mathbf{x}') d\mathbf{x}'. \end{aligned} \quad (45)$$

where

$$\begin{aligned} \tau_{p,q}^{\text{new}}(\mathbf{x}) &= -s\Lambda \int_D G_{p,q,i,i}^{\tau,h}(\mathbf{x}-\mathbf{x}') \chi^\Lambda(\mathbf{x}') \tau_{k,k}^{\text{inc}}(\mathbf{x}') d\mathbf{x}' \\ &\quad - 2sM \int_D G_{p,q,i,j}^{\tau,h}(\mathbf{x}-\mathbf{x}') \chi^M(\mathbf{x}') \tau_{i,j}^{\text{inc}}(\mathbf{x}') d\mathbf{x}' \\ &\quad + \frac{s}{c_s} \int_D G_{p,q,k}^{\tau,f}(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') u_k^{\text{inc}}(\mathbf{x}') d\mathbf{x}', \end{aligned} \quad (46)$$

$$\begin{aligned} u_r^{\text{new}}(\mathbf{x}) &= \rho c_s s \Lambda \int_D G_{r,i,i}^{v,h}(\mathbf{x}-\mathbf{x}') \chi^\Lambda(\mathbf{x}') \tau_{k,k}^{\text{inc}}(\mathbf{x}') d\mathbf{x}' \\ &\quad + 2\rho c_s s M \int_D G_{r,i,j}^{v,h}(\mathbf{x}-\mathbf{x}') \chi^M(\mathbf{x}') \tau_{i,j}^{\text{inc}}(\mathbf{x}') d\mathbf{x}' \\ &\quad - s\rho \int_D G_{r,k}^{v,f}(\mathbf{x}-\mathbf{x}') \chi^\rho(\mathbf{x}') u_k^{\text{inc}}(\mathbf{x}') d\mathbf{x}'. \end{aligned} \quad (47)$$

Therefore, after solving for  $\tau_{i,j}^{\text{sct}}(\mathbf{x})$  and  $u_k^{\text{sct}}(\mathbf{x})$  in Eq.(44) and Eq.(45), we obtain the total wavefields through the following relations:

$$\tau_{i,j}(\mathbf{x}) = \tau_{i,j}^{\text{sct}}(\mathbf{x}) + \tau_{i,j}^{\text{inc}}(\mathbf{x}), \quad \mathbf{x} \in D, \quad (48)$$

$$u_k(\mathbf{x}) = u_k^{\text{sct}}(\mathbf{x}) + u_k^{\text{inc}}(\mathbf{x}), \quad \mathbf{x} \in D, \quad (49)$$

### 3.6 Scattered particle velocities at the receivers

After obtaining the stress tensor and the particle velocity vector inside test domain  $D$ , from Eq.(31), the scattered field of the particle velocity at the receivers (i.e.,  $\mathbf{x} \notin D$ ) can be calculated as follows:

$$\begin{aligned}
& v_r^{\text{sct}}(\mathbf{x}) \\
&= \frac{\lambda}{2\mu} \frac{s}{\rho c_p^2} \int_D \partial_r G_p(\mathbf{x} - \mathbf{x}') \chi^\Lambda(\mathbf{x}') \tau_{k,k}(\mathbf{x}') d\mathbf{x}' - \frac{\lambda}{2\mu} \frac{s}{\rho c_p^2} \int_D \partial_r G_p(\mathbf{x} - \mathbf{x}') \chi^M(\mathbf{x}') \tau_{k,k}(\mathbf{x}') d\mathbf{x}' \\
&\quad - \frac{1}{\rho s} \int_D \partial_r \partial_i \partial_j (G_p - G_s)(\mathbf{x} - \mathbf{x}') \chi^M(\mathbf{x}') \tau_{i,j}(\mathbf{x}') d\mathbf{x}' - \frac{s}{\rho c_s^2} \int_D \partial_j G_s(\mathbf{x} - \mathbf{x}') \chi^M(\mathbf{x}') \tau_{r,j}(\mathbf{x}') d\mathbf{x}' \\
&\quad - \frac{s^2}{\rho c_s^3} \int_D G_s(\mathbf{x} - \mathbf{x}') \chi^\rho(\mathbf{x}') u_r(\mathbf{x}') d\mathbf{x}' - \frac{1}{\rho c_s} \int_D \partial_r \partial_k (G_p - G_s)(\mathbf{x} - \mathbf{x}') \chi^\rho(\mathbf{x}') u_k(\mathbf{x}') d\mathbf{x}', \quad (50)
\end{aligned}$$

where the partial derivatives of Helmholtz Green's function are calculated analytically, see [1].

## 4 Numerical treatment

### 4.1 Discretization procedure

We assume that the domain  $D$  which contains the scatterers is a rectangular domain with boundaries along the  $x_1$ ,  $x_2$ , and  $x_3$  directions. A Cartesian coordinate system is centered in  $D$ . The domain  $D$  may be chosen quite large to ensure inclusion of the scattering objects but this incurs a computational price.

We discretize the domain  $D$  in a rectangular mesh. The mesh is uniformly spaced in the  $x_1$ ,  $x_2$ , and  $x_3$  direction. The rectangular subdomains with widths of  $\Delta x_1$  in the  $x_1$  direction,  $\Delta x_2$  in the  $x_2$  direction, and  $\Delta x_3$  in the  $x_3$  direction are given by

$$\begin{aligned}
D_{m,n,l} = \{ & (x_1, x_2, x_3) \in \mathcal{R}^3 \mid x_{1;m} - \frac{1}{2}\Delta x_1 < x_1 < x_{1;m} + \frac{1}{2}\Delta x_1, \\
& x_{2;n} - \frac{1}{2}\Delta x_2 < x_2 < x_{2;n} + \frac{1}{2}\Delta x_2, x_{3;l} - \frac{1}{2}\Delta x_3 < x_3 < x_{3;l} + \frac{1}{2}\Delta x_3 \}, \quad (51)
\end{aligned}$$

where

$$x_{1;m} = x_{1;1/2} + (m - \frac{1}{2})\Delta x_1, \quad m = 1, \dots, M, \quad (52)$$

$$x_{2;n} = x_{2;1/2} + (n - \frac{1}{2})\Delta x_2, \quad n = 1, \dots, N, \quad (53)$$

$$x_{3;l} = x_{3;1/2} + (l - \frac{1}{2})\Delta x_3, \quad l = 1, \dots, L, \quad (54)$$

in which  $x_{1;1/2}$  is the lower  $x_1$  bound of domain  $D$ ,  $x_{2;1/2}$  is its lower  $x_2$  bound, and  $x_{3;1/2}$  is its lower  $x_3$  bound.

In each subdomain  $D_{m,n,l}$  with center points at  $(x_{1;m}, x_{2;n}, x_{3;l})$ , we assume the material contrasts  $\chi^\Lambda$ ,  $\chi^M$  and  $\chi^\rho$  to be constant, with value the same as the value at the center point

$$\chi_{m,n,l}^\beta = \chi^\beta(x_{1;m}, x_{2;n}, x_{3;l}), \quad \text{where } \beta \in \{\Lambda, M, \rho\}. \quad (55)$$

In view of the present of spatial differentiations in Eq.(61), the boundary of the domain  $D$  is chosen to be lied completely outside the scattering objects, and hence

$$\chi_{1,n,l}^\beta = 0, \quad \chi_{M,n,l}^\beta = 0, \quad \forall n, \forall l, \quad (56)$$

$$\chi_{m,1,l}^\beta = 0, \quad \chi_{m,N,l}^\beta = 0, \quad \forall m, \forall l, \quad (57)$$

$$\chi_{m,n,1}^\beta = 0, \quad \chi_{m,n,L}^\beta = 0, \quad \forall m, \forall n. \quad (58)$$

Now using the spatial discretization grid described above, we are able to discretize those continuous quantities. For example,  $\tau_{p,q;m,n,l}$  is defined as

$$\tau_{p,q;m,n,l} = \tau_{p,q}(x_{1;m}, x_{2;n}, x_{3;l}). \quad (59)$$

Therefore, Eq.(32) and Eq.(33) are discretized as

$$\tau_{p,q;m,n,l}^{inc} = \tau_{p,q;m,n,l} + B_{p,q;m,n,l}^{\tau,\Lambda} + B_{p,q;m,n,l}^{\tau,M} + B_{p,q;m,n,l}^{\tau,\rho}, \quad (60)$$

$$\rho c_s v_{r;m,n,l}^{inc} = u_{r;m,n,l} + B_{r;m,n,l}^{u,\Lambda} + B_{r;m,n,l}^{u,M} + B_{r;m,n,l}^{u,\rho}, \quad (61)$$

for  $m = 1, \dots, M$ ,  $n = 1, \dots, N$ , and  $l = 1, \dots, L$ .

## 4.2 Weakening procedure

Next, the continuous representation of the vector potentials in Eq.(40)-Eq.(41) ought to be discretized in the similar way. However, in order to cope with the singularity of the Green function, we take the spherical mean of the normalized vector potential in the Cartesian space. We integrate each vector potential over a spherical domain [22,23] in the Cartesian space with center at the point  $(x_{1;m}, x_{2;n}, x_{3;l})$  with radius  $\frac{1}{2}\Delta x = \frac{1}{2}\min(\Delta x_1, \Delta x_2, \Delta x_3)$ . The results are divided by the volume of the spherical domain with radius  $\frac{1}{2}\Delta x$ . For instance,

$$\begin{aligned}
& A^{P,\Lambda}(x_{1;m}, x_{2;n}, x_{3;l}) \\
&= \frac{\int_{|\mathbf{x}''| < 1/2\Delta x} A^{P,\Lambda}(x_{1;m} + x_1'', x_{2;n} + x_2'', x_{3;l} + x_3'') dx_1'' dx_2'' dx_3''}{\int_{|\mathbf{x}''| < 1/2\Delta x} dx_1'' dx_2'' dx_3''} \\
&= \int_D \mathcal{G}^P(x_{1;m} - x_1', x_{2;n} - x_2', x_{3;l} - x_3') \chi^\Lambda(x_1', x_2', x_3') \tau_{k,k}(x_1', x_2', x_3') dx_1' dx_2' dx_3',
\end{aligned} \tag{62}$$

where we have interchanged the order of integrations, such that

$$\begin{aligned}
& \mathcal{G}^P(x_1, x_2, x_3) \\
&= \frac{\int_{[(x_1'')^2 + (x_2'')^2 + (x_3'')^2]^{\frac{1}{2}} < \frac{1}{2}\Delta x} G_p(x_1 + x_1'', x_2 + x_2'', x_3 + x_3'') dx_1'' dx_2'' dx_3''}{\int_{[(x_1'')^2 + (x_2'')^2 + (x_3'')^2]^{\frac{1}{2}} < \frac{1}{2}\Delta x} dx_1'' dx_2'' dx_3''} \\
&= \begin{cases} \frac{[1 + \frac{s}{2c_p}\Delta x] \exp(-\frac{s}{2c_p}\Delta x) - 1}{-\frac{s^2}{6c_p^2}\pi\Delta x^3}, & R = 0, \\ \frac{\exp\left[-\frac{s}{c_p}R\right] \left[\frac{\sinh(-\frac{s}{2c_p}\Delta x)}{-\frac{s}{2c_p}\Delta x} - \cosh(\frac{s}{2c_p}\Delta x)\right]}{-\frac{s^2}{3c_p^2}\pi\Delta x^2 R}, & R > \frac{1}{2}\Delta x, \end{cases} \tag{63}
\end{aligned}$$

in which the distance function  $R$  is given by

$$R(x_1, x_2, x_3) = (x_1^2 + x_2^2 + x_3^2)^{\frac{1}{2}}. \tag{64}$$

After this weakening procedure, we are now able to compute the integral over  $D$  in Eq.(62) numerically. We approximate the integral in Eq.(62) using a midpoint rule. We then arrive at

$$A_{m,n,l}^{\text{p},\Lambda} = A^{\text{p},\Lambda}(x_1; m, x_2; n, x_3; l) = \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \mathcal{G}_{m-m', n-n', l-l'}^{\text{p}} \chi_{m', n', l'}^{\Lambda} \tau_{k,k; m', n', l'}, \quad (65)$$

for  $m = -1, \dots, M + 2$ ,  $n = -1, \dots, N + 2$ , and  $l = -1, \dots, L + 2$ , where

$$\mathcal{G}_{m-m', n-n', l-l'}^{\text{p}} = \mathcal{G}^{\text{p}}(x_1; m - x_1; m', x_2; n - x_2; n', x_3; l - x_3; l'). \quad (66)$$

Hence, following the above discretization procedure, all the vector potentials in Eq.(40)-Eq.(41) are discretized into totally 19 convolutions in the similar form of Eq.(65). These convolutions can be calculated efficiently using FFT routine, see [6].

Finally, we are able to write out the complete discretized form of Eq.(60) and Eq.(61). Here we list one component of  $B_{p,q; m, n, l}^{\tau, \Lambda}$  as illustration, the others can be found in Appendix (A):

$$B_{1,1; m, n, l}^{\tau, \Lambda} = \frac{\lambda}{\rho c_p^2} \chi_{m, n, l}^{\Lambda} (\tau_{1,1; m, n, l} + \tau_{2,2; m, n, l} + \tau_{3,3; m, n, l}) + \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m, n, l}^{\text{p}, \Lambda} + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} (A_{m-1, n, l}^{\text{p}, \Lambda} - 2A_{m, n, l}^{\text{p}, \Lambda} + A_{m+1, n, l}^{\text{p}, \Lambda}). \quad (67)$$

### 4.3 Linear equation solvers and pre-conditioners

Since the linear equation system of Eq.(60) and Eq.(61) has  $9 \times M \times N \times L$  unknowns and the matrix of operation is highly full, iterative linear equation solvers will be more suitable than direct solvers. However, among the various iterative linear equation solvers, those conjugate gradient techniques are more attractive in our problem. By using these techniques, the matrix doesn't need to be stored, the memory cost is therefore minimized.

Since the matrix of operation here is not positive definite, we first choose to use the so-called CGNR method, due to its well-known versatility and stability. More precisely, the adjoint operator of the given linear operator is applied as a pre-conditioner in the scheme of pre-conditioned Conjugate Gradient

method, so that the matrix of operation becomes positive definite. However, the condition number of the actual linear operator is twice of the original one, which make the convergence rate slower.

Besides the CGNR technique, BiCGStab is another attractive iterative linear equation solver [15]. However it suffers a lot from irregular convergence behavior when the matrix is ill-conditioned. To improve the performance of those linear equation solvers, we propose another two types of pre-conditioners: diagonal matrix pre-conditioner and EBA pre-conditioner. They are shown to be helpful in the numerical tests.

#### 4.3.1 Adjoint operator and its explicit expression

In order to implement the so-called CGNR linear equation solver, we first have to write out the explicit expression of its adjoint operator. The adjoint operators  $\mathcal{K}^*$  is defined through the relation

$$\langle r_{p,q}, \mathcal{K}s_{p,q} \rangle_D = \langle \mathcal{K}^*r_{p,q}, s_{p,q} \rangle_D, \quad (68)$$

where  $r_{p,q}$  and  $s_{p,q}$  are both in the same tensor space, in domain  $D$ . Note that  $s_{0,1}-s_{0,3}$  is referred to  $u_1-u_3$ , and other  $s_{p,q}$ 's are referred to the six components of  $\tau_{p,q}$ . The inner product on  $D$  is therefore defined as follows:

$$\langle a_{p,q}, b_{p,q} \rangle_D = \sum_{(p,q) \in \Phi} \sum_{m=1}^M \sum_{n=1}^N \sum_{l=1}^L a_{p,q;m,n,l} \bar{b}_{p,q;m,n,l}, \quad (69)$$

where  $\Phi = \{(1, 1), (2, 2), (3, 3), (1, 2), (1, 3), (2, 3), (0, 1), (0, 2), (0, 3)\}$ .

These definitions allow us to get the explicit expression of  $\mathcal{K}^*$ . Here we list only one component of  $\mathcal{K}^*r_{p,q}$  as illustration:

$$\begin{aligned} (\mathcal{K}^*r_{p,q})_{1,1;m,n,l} &= \frac{\overline{\lambda}}{\rho c_p^2} \overline{\chi_{m,n,l}^\Lambda} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\ &\quad - \overline{\chi_{m,n,l}^M} r_{1,1;m,n,l} - \left( \frac{\overline{\lambda}}{\rho c_p^2} \right) \overline{\chi_{m,n,l}^M} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\ &\quad + \overline{\chi_{m,n,l}^\Lambda} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{m',n',l'}^{\text{p},\Lambda} \\ &\quad - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{1,1;m',n',l'}^{\text{p},M} \end{aligned}$$

$$-\overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{1,1;m',n',l'}^{s,M}, \quad (70)$$

for  $m = 1, \dots, M$ ,  $n = 1, \dots, N$ , and  $l = 1, \dots, L$ . Here,  $F_{m,n,l}^{p,\Lambda}$ ,  $F_{1,1;m,n,l}^{p,\Lambda}$  and  $F_{1,1;m,n,l}^{s,\Lambda}$  are related to the finite difference operators in  $\mathcal{K}$ . We also list one as illustration:

$$\begin{aligned} F_{m,n,l}^{p,\Lambda} = & \overline{\left( \frac{\lambda}{\rho c_p^2} \right)} \left[ \overline{\left( \frac{\lambda s^2}{2\mu c_p^2} \right)} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{2,2;m,n,l}) \right. \\ & + \frac{1}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\ & + \frac{1}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\ & + \frac{1}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{2,2;m,n,l} + r_{2,2;m,n,l+1}) \\ & + \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\ & + \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\ & + \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n+1,l-1} - r_{2,3;m,n-1,l+1} + r_{2,3;m,n+1,l+1}) \\ & - \overline{\left( \frac{s\rho c_s}{2\mu} \right)} \frac{1}{2\Delta x_1} (r_{1;m-1,n,l} - r_{1;m+1,n,l}) \\ & - \overline{\left( \frac{s\rho c_s}{2\mu} \right)} \frac{1}{2\Delta x_2} (r_{2;m,n-1,l} - r_{2;m,n+1,l}) \\ & \left. - \overline{\left( \frac{s\rho c_s}{2\mu} \right)} \frac{1}{2\Delta x_3} (r_{3;m,n,l-1} - r_{3;m,n,l+1}) \right], \quad (71) \end{aligned}$$

Please see Appendix (B) for the complete expression of the adjoint operator.

#### 4.3.2 Diagonal pre-conditioner

Consider the linear operator  $\mathcal{K}$  as a matrix and denote its diagonal matrix as  $\mathcal{D}$ , we are interested in using  $\mathcal{D}^{-1}$  as a pre-conditioner. In other words, instead of solving  $\mathcal{K}s_{p,q} = s_{p,q}^{inc}$ , we are solving  $\mathcal{D}^{-1}\mathcal{K}s_{p,q} = \mathcal{D}^{-1}s_{p,q}^{inc}$ . While the complete explicit expression of  $\mathcal{D}$  can be found in Appendix (C), the first component of  $\mathcal{D}$  is illustrated below:

$$\begin{aligned}
\mathcal{D}_{1,1;m,n,l} = & 1 + \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^\Lambda + \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^\Lambda \\
& + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\Lambda (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
& - \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^M \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
& - 2 \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s) \\
& - \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_1)^2} \left[ \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^p - 2\mathcal{G}_{-1,0,0}^p + \mathcal{G}_{0,0,0}^p) \right. \\
& - 2 \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
& \left. + \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - 2\mathcal{G}_{1,0,0}^p + \mathcal{G}_{2,0,0}^p) \right] \\
& + \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_1)^2} \left[ \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^s - 2\mathcal{G}_{-1,0,0}^s + \mathcal{G}_{0,0,0}^s) \right. \\
& - 2 \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s) \\
& \left. + \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - 2\mathcal{G}_{1,0,0}^s + \mathcal{G}_{2,0,0}^s) \right], \tag{72}
\end{aligned}$$

### 4.3.3 EBA pre-conditioner

One may think the inverse of a good approximation of the linear operator  $\mathcal{K}$  might be a better pre-conditioner. Since the Extended Born Approximation (known as EBA) technique has shown to be excellent in some other integral equation problems [12]. Therefore, we first investigate its behavior in our problem, and then propose to use it as a pre-conditioner.

The idea of EBA is to use the following approximation for the internal wavefield inside the integrand of the equations:

$$\tau_{i,j}(\mathbf{x}') \approx \tau_{i,j}(\mathbf{x}), \quad \mathbf{x} \in D, \tag{73}$$

$$u_k(\mathbf{x}') \approx u_k(\mathbf{x}), \quad \mathbf{x} \in D, \tag{74}$$

where we have approximated the internal wavefield by its first term in its Taylor series expansion, hence, under this localization approximation, Eq.(32) and Eq.(33) are represented by

$$\begin{aligned}
\tau_{p,q}^{\text{inc}}(\mathbf{x}) &= \tau_{p,q}(\mathbf{x}) + s\Lambda \int_D G_{p,q,i,i}^{\tau,h}(\mathbf{x}-\mathbf{x}')\chi^\Lambda(\mathbf{x}')d\mathbf{x}'\tau_{k,k}(\mathbf{x}) \\
&\quad + 2sM \int_D G_{p,q,i,j}^{\tau,h}(\mathbf{x}-\mathbf{x}')\chi^M(\mathbf{x}')d\mathbf{x}'\tau_{i,j}(\mathbf{x}) \\
&\quad - \frac{s}{c_s} \int_D G_{p,q,k}^{\tau,f}(\mathbf{x}-\mathbf{x}')\chi^\rho(\mathbf{x}')d\mathbf{x}'u_k(\mathbf{x}) \\
&= \tau_{p,q}(\mathbf{x}) + E_{p,q}^{\tau,\Lambda}(\mathbf{x})\tau_{k,k}(\mathbf{x}) + E_{p,q,i,j}^{\tau,M}(\mathbf{x})\tau_{i,j}(\mathbf{x}) + E_{p,q,k}^{\tau,\rho}(\mathbf{x})u_k(\mathbf{x}) \quad (75)
\end{aligned}$$

$$\begin{aligned}
\rho c_s v_r^{\text{inc}}(\mathbf{x}) &= u_r(\mathbf{x}) - \rho c_s s\Lambda \int_D G_{r,i,i}^{v,h}(\mathbf{x}-\mathbf{x}')\chi^\Lambda(\mathbf{x}')d\mathbf{x}'\tau_{k,k}(\mathbf{x}) \\
&\quad - 2\rho c_s sM \int_D G_{r,i,j}^{v,h}(\mathbf{x}-\mathbf{x}')\chi^M(\mathbf{x}')d\mathbf{x}'\tau_{i,j}(\mathbf{x}) \\
&\quad + s\rho \int_D G_{r,k}^{v,f}(\mathbf{x}-\mathbf{x}')\chi^\rho(\mathbf{x}')d\mathbf{x}'u_k(\mathbf{x}) \\
&= u_r(\mathbf{x}) + E_r^{u,\Lambda}(\mathbf{x})\tau_{k,k}(\mathbf{x}) + E_{r,i,j}^{u,M}(\mathbf{x})\tau_{i,j}(\mathbf{x}) + E_{r,k}^{u,\rho}(\mathbf{x})u_k(\mathbf{x}) \quad (76)
\end{aligned}$$

where

$$E_{p,q}^{\tau,\Lambda}(\mathbf{x}) = \frac{\lambda}{2\mu} \left\{ \delta_{p,q} \left[ \frac{2c_s^2}{c_p^2} \chi^\Lambda(\mathbf{x}) + \frac{\lambda s^2}{\rho c_p^4} Y^{\text{p},\Lambda}(\mathbf{x}) \right] + \frac{2c_s^2}{c_p^2} \partial_p \partial_q Y^{\text{p},\Lambda}(\mathbf{x}) \right\} \quad (77)$$

is a 6-by-3 matrix,

$$\begin{aligned}
E_{p,q,i,j}^{\tau,M}(\mathbf{x}) &= -\frac{\lambda}{2\mu} \left\{ \delta_{p,q} \left[ \frac{2c_s^2}{c_p^2} \delta_{i,j} \chi^M(\mathbf{x}) + \frac{\lambda s^2}{\rho c_p^4} \delta_{i,j} Y^{\text{p},M}(\mathbf{x}) + \frac{2c_s^2}{c_p^2} \partial_i \partial_j Y^{\text{p},M}(\mathbf{x}) \right] \right. \\
&\quad \left. + \frac{2c_s^2}{c_p^2} \delta_{i,j} \partial_p \partial_q Y^{\text{p},M}(\mathbf{x}) \right\} - \chi^M(\mathbf{x}) \delta_{p,i} \delta_{q,j} \\
&\quad - \left[ \delta_{q,i} \partial_p \partial_j Y^{\text{s},M}(\mathbf{x}) + \delta_{p,i} \partial_q \partial_j Y^{\text{s},M}(\mathbf{x}) \right] - \frac{2c_s^2}{s^2} \partial_p \partial_q \partial_i \partial_j (Y^{\text{p},M} - Y^{\text{s},M})(\mathbf{x}), \quad (78)
\end{aligned}$$

is a 6-by-6 matrix,

$$\begin{aligned}
E_{p,q,k}^{\tau,\rho}(\mathbf{x}) &= -\frac{\lambda}{\rho c_p^2} \frac{s}{c_s} \delta_{p,q} \partial_k Y^{\text{p},\rho}(\mathbf{x}) - \frac{s}{c_s} [\delta_{q,k} \partial_p Y^{\text{s},\rho}(\mathbf{x}) + \delta_{p,k} \partial_q Y^{\text{s},\rho}(\mathbf{x})] \\
&\quad - \frac{2\mu}{s\rho c_s} \partial_p \partial_q \partial_k (Y^{\text{p},\rho} - Y^{\text{s},\rho})(\mathbf{x}), \tag{79}
\end{aligned}$$

is a 6-by-3 matrix,

$$E_r^{u,\Lambda}(\mathbf{x}) = -\frac{\lambda s c_s}{2\mu c_p^2} \partial_r Y^{\text{p},\Lambda}(\mathbf{x}), \tag{80}$$

is a 3-by-3 matrix,

$$\begin{aligned}
E_{r,i,j}^{u,M}(\mathbf{x}) &= \frac{\lambda s c_s}{2\mu c_p^2} \delta_{i,j} \partial_r Y^{\text{p},M}(\mathbf{x}) + \frac{s\rho c_s}{\mu} \delta_{r,j} \partial_i Y^{\text{s},M}(\mathbf{x}) + \frac{c_s}{s} \partial_r \partial_i \partial_j (Y^{\text{p},M} - Y^{\text{s},M})(\mathbf{x}), \tag{81}
\end{aligned}$$

is a 3-by-6 matrix, and

$$E_{r,k}^{u,\rho}(\mathbf{x}) = \frac{s^2}{c_s^2} \delta_{r,k} Y^{\text{s},\rho}(\mathbf{x}) + \partial_r \partial_k (Y^{\text{p},\rho} - Y^{\text{s},\rho})(\mathbf{x}), \tag{82}$$

is a 3-by-3 matrix.

Here, we define

$$Y^{\gamma,\beta}(\mathbf{x}) = \int_D G_\gamma(\mathbf{x} - \mathbf{x}') \chi^\beta(\mathbf{x}') d\mathbf{x}', \tag{83}$$

where  $\gamma \in \{\text{p}, \text{s}\}$  and  $\beta \in \{\Lambda, M, \rho\}$ .

Explicitly, Eq.(75) and Eq.(76) can be written as follows:

$$\begin{aligned}
&\left[ \tau_{1,1}^{\text{inc}}(\mathbf{x}), \tau_{2,2}^{\text{inc}}(\mathbf{x}), \tau_{3,3}^{\text{inc}}(\mathbf{x}), \tau_{1,2}^{\text{inc}}(\mathbf{x}), \tau_{1,3}^{\text{inc}}(\mathbf{x}), \tau_{2,3}^{\text{inc}}(\mathbf{x}), u_1^{\text{inc}}(\mathbf{x}), u_2^{\text{inc}}(\mathbf{x}), u_3^{\text{inc}}(\mathbf{x}) \right]^T \\
&= \Gamma(\mathbf{x}) \cdot \left[ \tau_{1,1}(\mathbf{x}), \tau_{2,2}(\mathbf{x}), \tau_{3,3}(\mathbf{x}), \tau_{1,2}(\mathbf{x}), \tau_{1,3}(\mathbf{x}), \tau_{2,3}(\mathbf{x}), u_1(\mathbf{x}), u_2(\mathbf{x}), u_3(\mathbf{x}) \right]^T, \tag{84}
\end{aligned}$$

where  $T$  is the transpose notation, and  $\Gamma(\mathbf{x})$  is a 9-by-9 matrix defined as

$$\begin{aligned}
\Gamma(\mathbf{x}) = \mathbf{I}_{9 \times 9} + & \begin{bmatrix} E^{\tau, \Lambda}(\mathbf{x}) & \mathbf{0}_{6 \times 6} \\ \mathbf{0}_{3 \times 3} & \mathbf{0}_{3 \times 6} \end{bmatrix} + \begin{bmatrix} E^{\tau, M}(\mathbf{x}) & \mathbf{0}_{6 \times 3} \\ \mathbf{0}_{3 \times 6} & \mathbf{0}_{3 \times 3} \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{6 \times 6} & E^{\tau, \rho}(\mathbf{x}) \\ \mathbf{0}_{3 \times 6} & \mathbf{0}_{3 \times 3} \end{bmatrix} \\
& + \begin{bmatrix} \mathbf{0}_{6 \times 3} & \mathbf{0}_{6 \times 6} \\ E^{u, \Lambda}(\mathbf{x}) & \mathbf{0}_{3 \times 6} \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{6 \times 6} & \mathbf{0}_{6 \times 3} \\ E^{u, M}(\mathbf{x}) & \mathbf{0}_{3 \times 3} \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{6 \times 6} & \mathbf{0}_{6 \times 3} \\ \mathbf{0}_{3 \times 6} & E^{u, \rho}(\mathbf{x}) \end{bmatrix} \quad (85)
\end{aligned}$$

Therefore, following the same discretization procedure, we are able to implement the EBA operator  $\Gamma$ , and use its inverse operator as a pre-conditioner. In other words, instead of solving  $\mathcal{K}_{s,p,q} = s_{p,q}^{inc}$ , we are solving  $\Gamma^{-1} \mathcal{K}_{s,p,q} = \Gamma^{-1} s_{p,q}^{inc}$ .

#### 4.4 Discretized integral representation

Using the same discretization procedure, the scattered field of particle velocity in Eq.(50) can be represented as follows:

$$\begin{aligned}
v_r^{sct}(x_1^R, x_2^R, x_3^R) = & \frac{\lambda}{2\mu} \frac{s}{\rho c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_r G_p(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^\Lambda \tau_{k,k;m',n',l'} \\
& - \frac{\lambda}{2\mu} \frac{s}{\rho c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_r G_p(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^M \tau_{k,k;m',n',l'} \\
& - \frac{1}{\rho s} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_r \partial_i \partial_j G_p(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^M \tau_{i,j;m',n',l'} \\
& + \frac{1}{\rho s} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_r \partial_i \partial_j G_s(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^M \tau_{i,j;m',n',l'} \\
& - \frac{s}{\rho c_s^2} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_j G_s(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^M \tau_{r,j;m',n',l'} \\
& - \frac{s^2}{\rho c_s^3} \Delta x_1 \Delta x_2 \Delta x_3
\end{aligned}$$

$$\begin{aligned}
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L G_s(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^\rho u_{r;m',n',l'} \\
& - \frac{1}{\rho c_s} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_r \partial_k G_p(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^\rho u_{k;m',n',l'} \\
& + \frac{1}{\rho c_s} \Delta x_1 \Delta x_2 \Delta x_3 \\
& \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \partial_r \partial_k G_s(x_1^R - x_{1;m'}, x_2^R - x_{2;n'}, x_3^R - x_{3;l'}) \chi_{m',n',l'}^\rho u_{k;m',n',l'} ,
\end{aligned} \tag{86}$$

where  $x_1^R$ ,  $x_2^R$  and  $x_3^R$  are the receiver spatial positions and they are located outside the computational domain  $D$ .

## 5 Numerical results

Throughout our numerical tests in this section, the background mass always has a compressional speed of 1500 m/s and a shear speed of 1000 m/s. The density is 2000 kg/m<sup>3</sup>. The point excitation force employed is directed in the negative vertical z-direction located at (0, 0, 2)m. There are 30 receivers equally arranged along the line from (-3.0, 0, 1.5)m to (3.0, 0, 1.5)m. The frequency of operation is 1.5 kHz.

### 5.1 Example I

The first model we consider is an object with dimension 0.8m by 0.8m by 0.8m as shown in Fig.(2). The object has a density of 3000 kg/m<sup>3</sup>, a compressional speed of 3000m/s and a shear speed of 2000m/s. The computational domain  $D$  is of dimension 1.0 m by 1.0 m by 1.0 m, and its center is located at (0, 0, 0)m.

First, we do the consistency test as we refine the grids. Fig.(3) shows us the scattered particle velocities at the receivers when the number of computational points along each axis is 10, 20, 40 and 62, respectively. The picture shows that the scattered particle velocities convergence as we refine the grids. The following table shows the convergence history of the consistency test, where the benchmark fields are calculated from the grids which have 62 computational

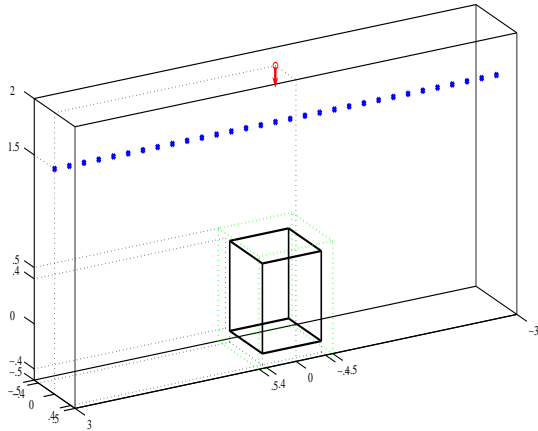


Fig. 2. The configuration for example I.

points along each axis. Therefore, we would claim that this algorithm are of order 2 in terms of convergence rate.

N	Relative Error in $v_1^{sct}$	Order	Relative Error in $v_3^{sct}$	Order
10	0.91169		0.91246	
20	0.29922	1.60732	0.35482	1.36263
40	0.07219	2.05135	0.08121	2.12729

Next, we take the reciprocity test as we change the positions of the source and some receivers. Here, the grids which have 40 computational points along each axis are used. The following table shows the results.

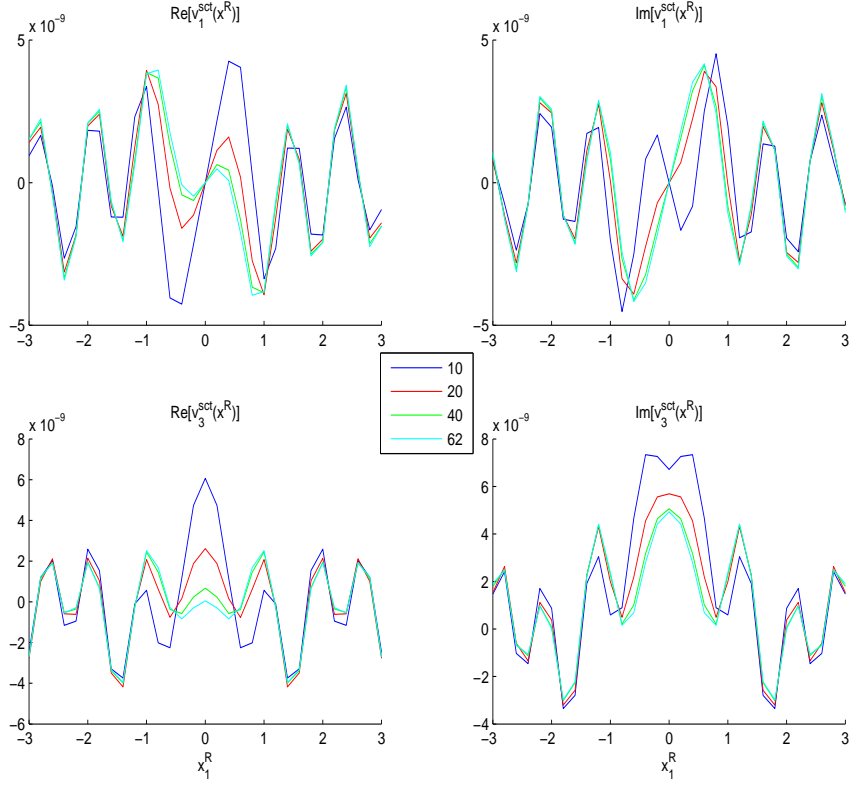


Fig. 3. Consistency test: example I.

Source		Receiver		Scattered field	
position	direction	position	direction	real	imaginary
(0, 0, 2)	z	(-3, 0, 1.5)	z	$-2.69839E - 09$	$1.79548E - 09$
(-3, 0, 1.5)	z	(0, 0, 2)	z	$-2.68349E - 09$	$1.79534E - 09$
(0, 0, 2)	z	(-3, 0, 1.5)	x	$1.52134E - 09$	$9.56448E - 10$
(-3, 0, 1.5)	x	(0, 0, 2)	z	$1.52854E - 09$	$9.76224E - 10$
(0, 0, 2)	z	(1.2, 0, 1.5)	z	$-2.23784E - 10$	$4.30452E - 09$
(1.2, 0, 1.5)	z	(0, 0, 2)	z	$-2.99350E - 10$	$4.39384E - 09$
(0, 0, 2)	z	(1.2, 0, 1.5)	x	$-7.94846E - 10$	$-2.84890E - 09$
(1.2, 0, 1.5)	x	(0, 0, 2)	z	$-7.74581E - 10$	$-2.86591E - 09$

To show that EBA is a good approximation to the integral equation operator, we compare the results among the following three methods: normalized integral equation of total field, extended Born approximation to the normal-

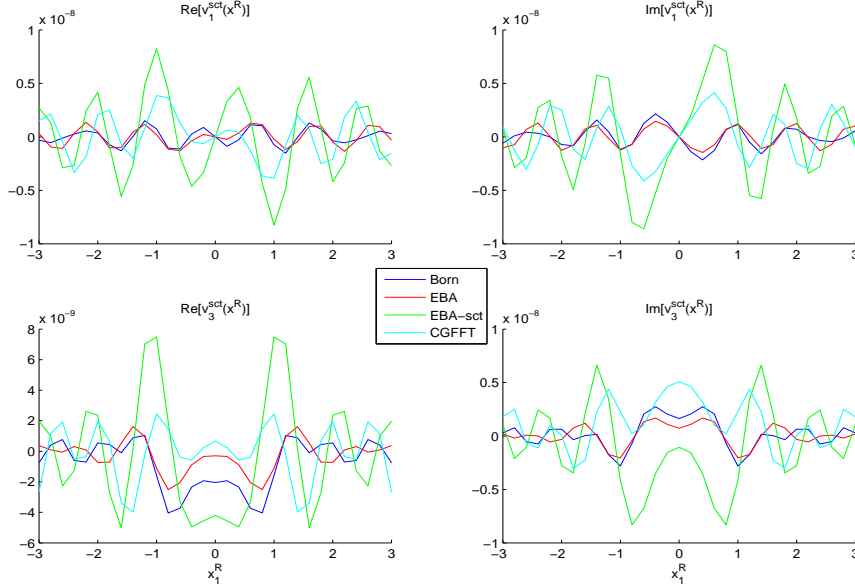


Fig. 4. The scattered field comparison among the four methods with frequency 1.5kHz: example I.

ized integral equation of total field, and extended Born approximation to the normalized integral equation of scattered field. Fig.(4) shows the comparison with frequency 1.5kHz, where there are 40 computational points along each axis. Fig.(5) shows the comparison with frequency 0.5kHz, where there are 20 computational points along each axis. Fig.(6) shows the comparison with frequency 0.1kHz, where there are 20 computational points along each axis.

As shown in the pictures, the EBA approximations are getting better when the frequency of operation decreases. The following Fig.(7) shows the comparison among the three linear system solvers: CG, CG with diagonal matrix preconditioner, BiCGStab with EBA preconditioner. The diagonal matrix preconditioner helps to improve the condition of the matrix, however, EBA preconditioner works better.

## 5.2 Example II

The second model we are interested in has two objects, which are of the same dimension of 0.5m by 0.5m by 0.5m, as shown in Fig.(8). The object on the left has a density of 3000 kg/m<sup>3</sup>, a compressional speed of 3000m/s and a shear speed of 1000m/s, while the object on the right has a density of 3000 kg/m<sup>3</sup>, a compressional speed of 1500m/s and a shear speed of 2000m/s. The computational domain is a cube of dimension 1.5 m by 1.5 m by 1.5 m centered

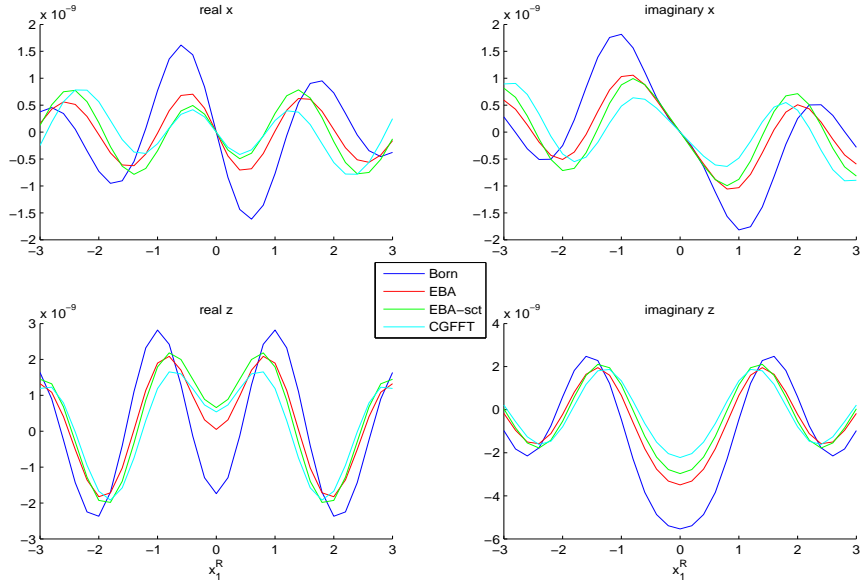


Fig. 5. The scattered field comparison among the four methods with frequency 0.5kHz: example I.

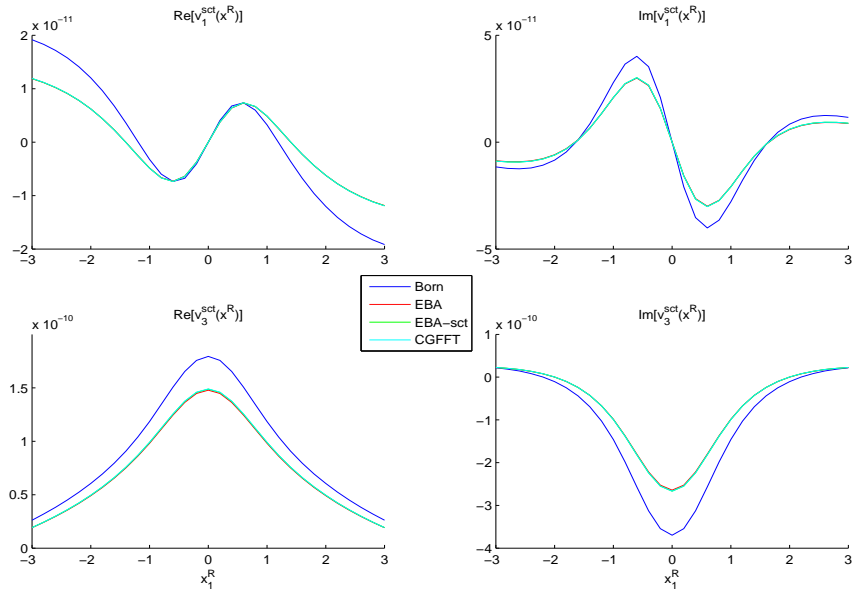


Fig. 6. The scattered field comparison among the four methods with frequency 0.5kHz: example I.

at  $(0, 0, 0)$ m.

We also do the consistency test first. Fig.(9) shows us the scattered particle velocities at the receivers when the number of computational points along each axis is 15, 30 and 60, respectively. The picture shows that the scattered

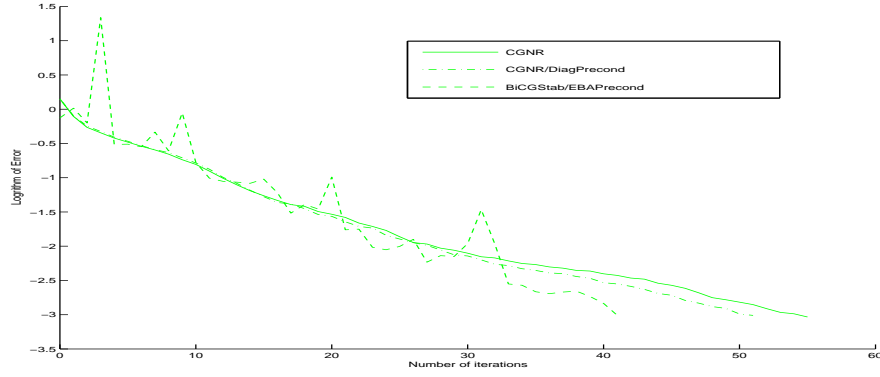


Fig. 7. The scattered field comparison among the three linear solvers with frequency 1.5kHz: example I.

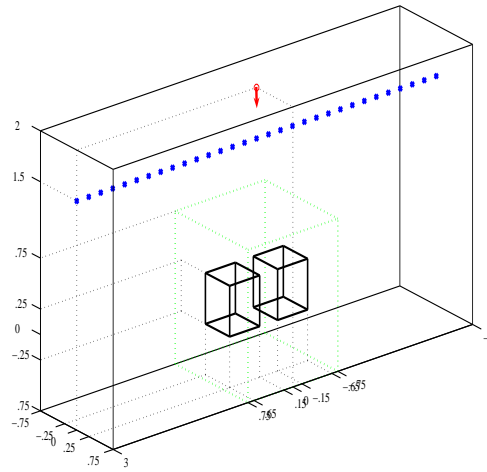


Fig. 8. The configuration for example II.

particle velocities convergence as the grids are refined. The following table shows the convergence history of the consistency test, where the benchmark fields are calculated from the grids which have 60 computational points along each axis. Therefore, we would claim that this algorithm are of order 2 in terms of convergence rate.

N	Relative Error in $v_1^{sct}$	Order	Relative Error in $v_3^{sct}$	Order
15	0.44879		0.39363	
30	0.14392	1.64069	0.11149	1.81990

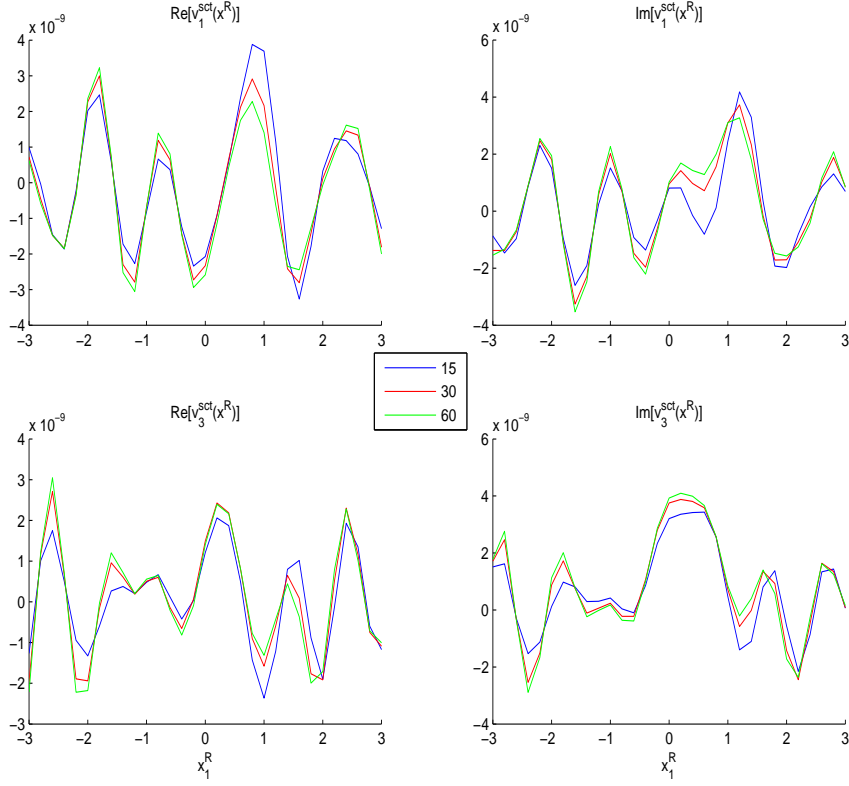


Fig. 9. Consistency Test: example II.

We take the reciprocity test as we change the positions of the source and some receivers. Here, the grids which have 30 computational points along each axis are used. The following table shows the results.

Source		Receiver		Scattered field	
position	direction	position	direction	real	imaginary
(0, 0, 2)	z	(-3, 0, 1.5)	z	$-1.96422E - 09$	$1.71150E - 09$
(-3, 0, 1.5)	z	(0, 0, 2)	z	$-2.03907E - 09$	$1.81249E - 09$
(0, 0, 2)	z	(-3, 0, 1.5)	x	$7.22419E - 10$	$-1.38030E - 09$
(-3, 0, 1.5)	x	(0, 0, 2)	z	$6.96509E - 10$	$-1.36840E - 09$
(0, 0, 2)	z	(1.2, 0, 1.5)	z	$-5.91748E - 10$	$-5.80956E - 10$
(1.2, 0, 1.5)	z	(0, 0, 2)	z	$-5.90618E - 10$	$-6.15488E - 10$
(0, 0, 2)	z	(1.2, 0, 1.5)	x	$-1.46338E - 10$	$3.73119E - 09$
(1.2, 0, 1.5)	x	(0, 0, 2)	z	$-2.12263E - 10$	$3.70624E - 09$

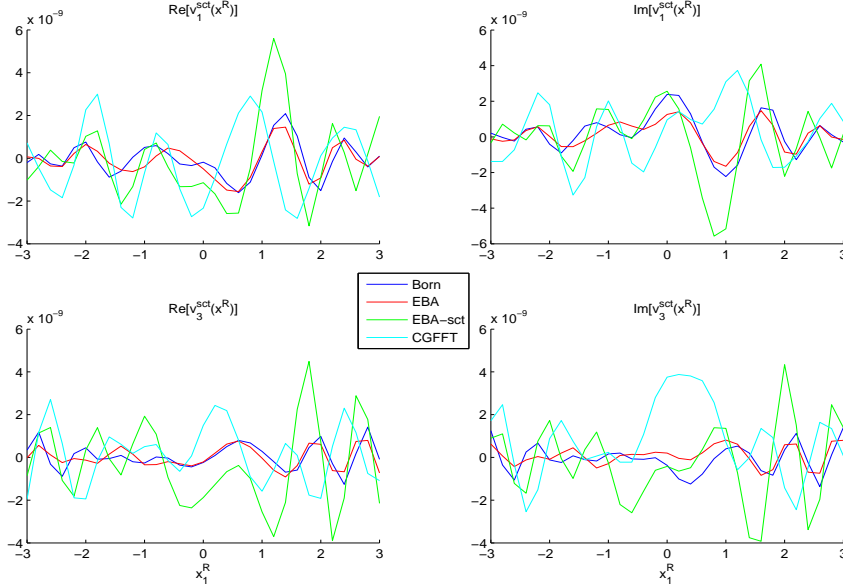


Fig. 10. The scattered field comparison among the four methods with frequency 1.5kHz: example II.

We compare the results among the following four methods: normalized integral equation of total field, Born approximation for the normalized integral equation of total field, extended Born approximation for the normalized integral equation of total field, and extended Born approximation for the normalized integral equation of scattered field. Fig.(10) shows the comparison with frequency 1.5kHz, where there are 30 computational points along each axis. Fig.(11) shows the comparison with frequency 0.5kHz, where there are 30 computational points along each axis. Fig.(12) shows the comparison with frequency 0.1kHz, where there are 20 computational points along each axis.

Once again, we can conclude from the above pictures that the EBA approximations are getting better when the frequency of operation decreases. Fig.(13) shows the comparison among the three linear system solvers as before. The diagonal matrix pre-conditioner works better while EBA pre-conditioner are the best.

### 5.3 Example III

Unlike the first two models where the objects have constant material properties, the third model we are testing has an object which is inhomogeneous in itself. The geometry of the third model is the same as the first model, as shown in Fig.(2), however, the material properties inside the object are given as follows:

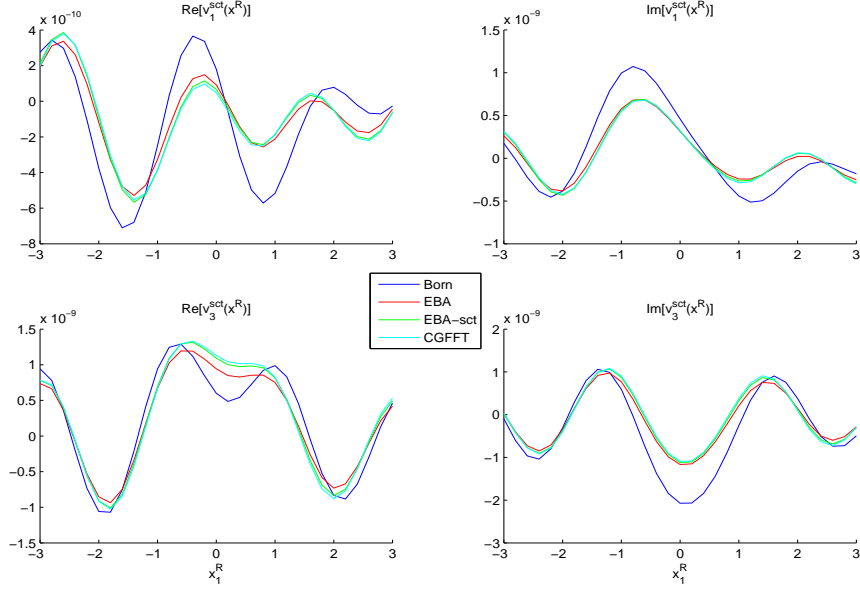


Fig. 11. The scattered field comparison among the four methods with frequency 0.5kHz: example II.

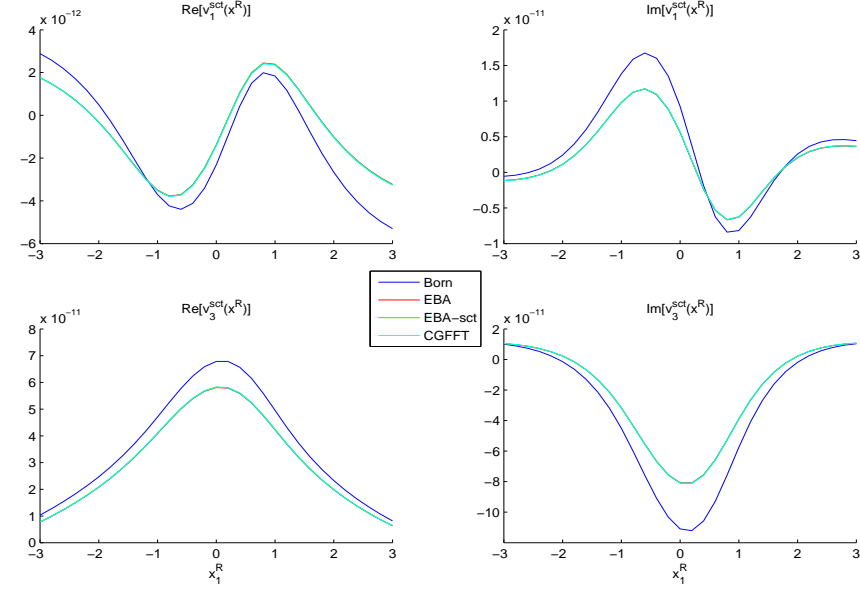


Fig. 12. The scattered field comparison among the four methods with frequency 0.5kHz: example II.

$$c_p = 1500 + 1500 \sin \left[ \frac{(x + 0.4)\pi}{0.8} \right] \sin \left[ \frac{(y + 0.4)\pi}{0.8} \right] \sin \left[ \frac{(z + 0.4)\pi}{0.8} \right]$$

$$c_s = 1000 + 1000 \sin \left[ \frac{(x + 0.4)\pi}{0.8} \right] \sin \left[ \frac{(y + 0.4)\pi}{0.8} \right] \sin \left[ \frac{(z + 0.4)\pi}{0.8} \right]$$

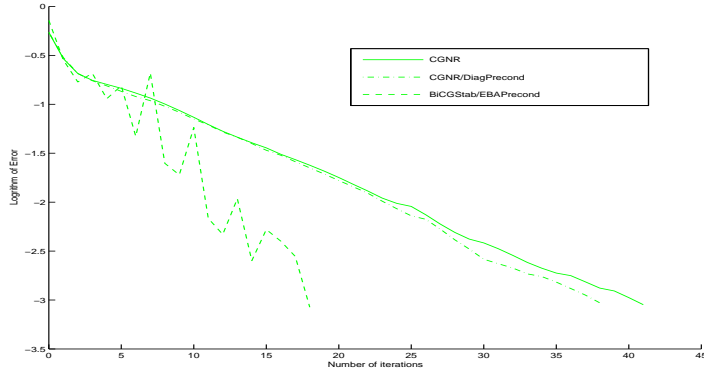


Fig. 13. The scattered field comparison among the three linear solvers with frequency 1.5kHz: example II.

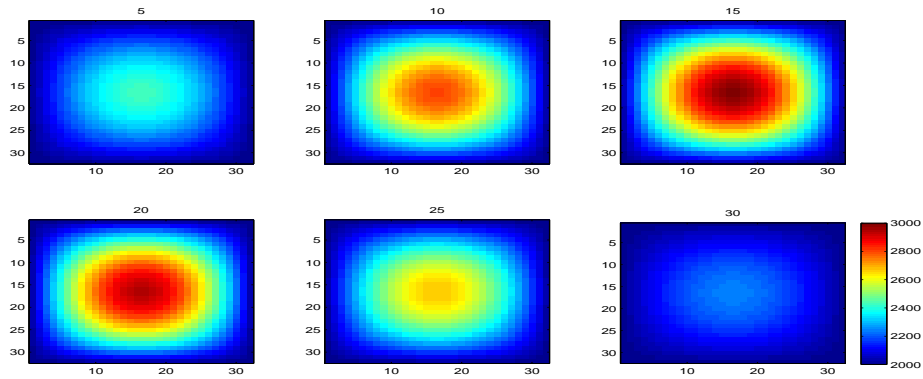


Fig. 14. The horizontal slice images for example III.

$$\rho = 2000 + 1000 \sin \left[ \frac{(x + 0.4)\pi}{0.8} \right] \sin \left[ \frac{(y + 0.4)\pi}{0.8} \right] \sin \left[ \frac{(z + 0.4)\pi}{0.8} \right] \quad (87)$$

Fig.(14) shows some horizontal slices of image of the density of the object. The slices for the  $c_p$  and  $c_s$  are similar to this.

We also do the consistency test first. Fig.(15) shows us the scattered particle velocities at the receivers when the number of computational points along each axis is 10, 20, 40 and 62, respectively. The picture shows that the scattered particle velocities convergence as the grids are refined. The following table shows the convergence history of the consistency test, where the benchmark fields are calculated from the grids which have 62 computational points along each axis. Therefore, we would claim that this algorithm are of order 2 in terms of convergence rate.

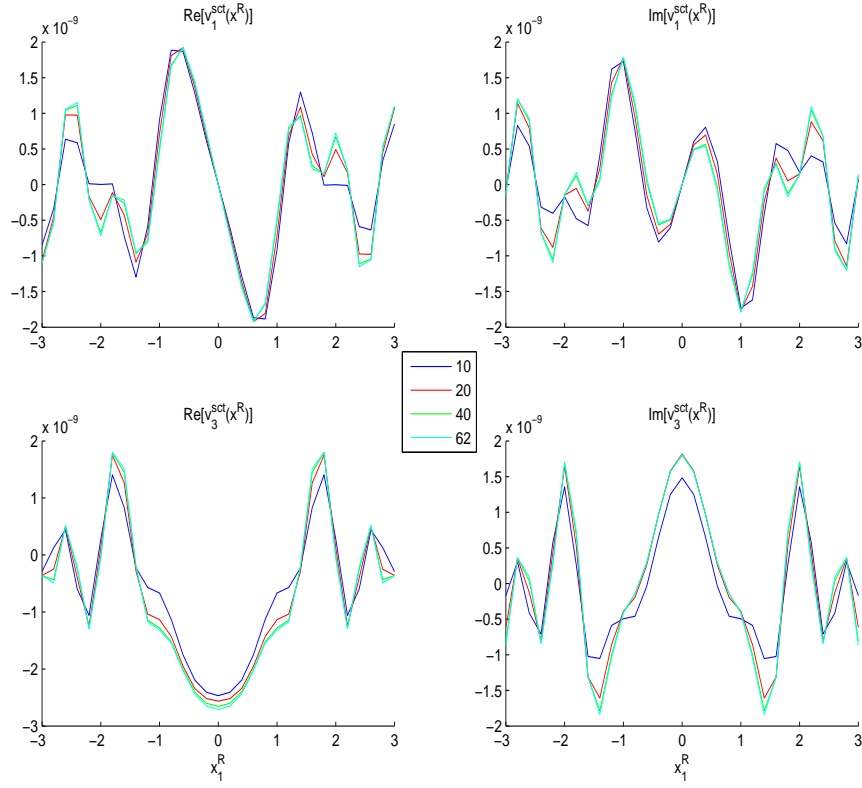


Fig. 15. Consistency test: example III.

N	Relative Error in $v_1^{sct}$	Order	Relative Error in $v_3^{sct}$	Order
10	0.39310		0.31772	
20	0.15304	1.36097	0.10925	1.54012
40	0.03404	2.16867	0.02797	1.96522

We take the reciprocity test as we change the positions of the source and some receivers. Here, the grids which have 40 computational points along each axis are used. The following table shows the results.

Source		Receiver		Scattered field	
position	direction	position	direction	real	imaginary
(0, 0, 2)	z	(-3, 0, 1.5)	z	$-3.57631E - 10$	$-6.15354E - 10$
(-3, 0, 1.5)	z	(0, 0, 2)	z	$-3.54839E - 10$	$-6.14178E - 10$
(0, 0, 2)	z	(-3, 0, 1.5)	x	$-1.07358E - 09$	$-8.06678E - 11$
(-3, 0, 1.5)	x	(0, 0, 2)	z	$-1.06841E - 09$	$-8.60503E - 11$
(0, 0, 2)	z	(1.2, 0, 1.5)	z	$-1.03777E - 09$	$-8.59058E - 10$
(1.2, 0, 1.5)	z	(0, 0, 2)	z	$-1.03271E - 09$	$-8.67737E - 10$
(0, 0, 2)	z	(1.2, 0, 1.5)	x	$6.86518E - 10$	$-1.42621E - 09$
(1.2, 0, 1.5)	x	(0, 0, 2)	z	$6.97678E - 10$	$-1.42766E - 09$

We compare the results among the following four methods: normalized integral equation of total field, Born approximation for the normalized integral equation of total field, extended Born approximation for the normalized integral equation of total field, and extended Born approximation for the normalized integral equation of scattered field. Fig.(16) shows the comparison with frequency 1.5kHz, where there are 40 computational points along each axis. Fig.(17) shows the comparison with frequency 0.5kHz, where there are 20 computational points along each axis. Fig.(18) shows the comparison with frequency 0.1kHz, where there are 20 computational points along each axis.

Once again, we can conclude from the above pictures that the EBA approximations are getting better when the frequency of operation decreases. Fig.(19) shows the comparison among the three linear system solvers as before. The diagonal matrix pre-conditioner works better while EBA pre-conditioner are the best.

## 6 Conclusions

In this paper, we developed an integral equation approach in terms of the stress tensor and the particle velocity. There is no differentiation operators working on the stress tensor/particle velocity inside the integral operators. All convolution operators are calculated efficiently using FFT routines. We used Conjugate Gradient (CGNR and BiCGStab) techniques to solve the linear system. We implemented both the diagonal matrix and the EBA as pre-

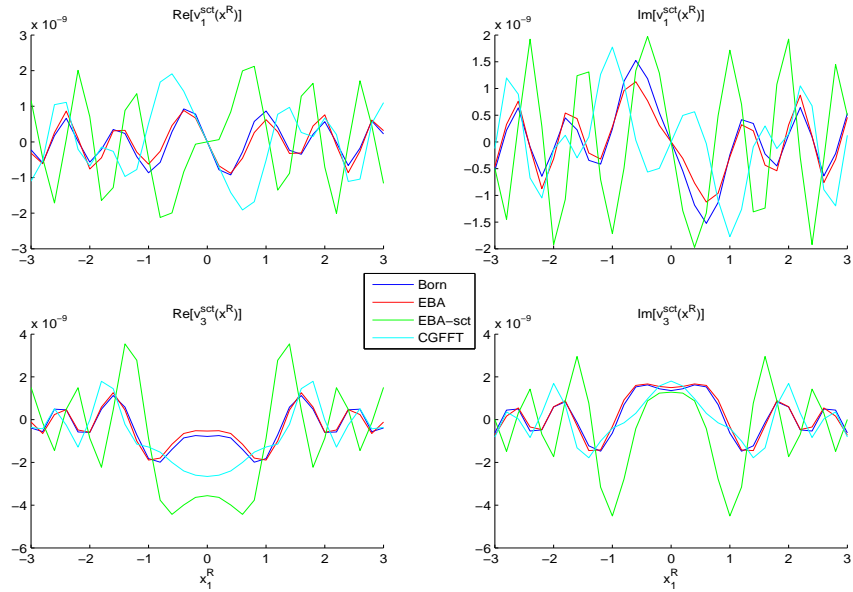


Fig. 16. The scattered field comparison among the four methods with frequency 1.5kHz: example III.

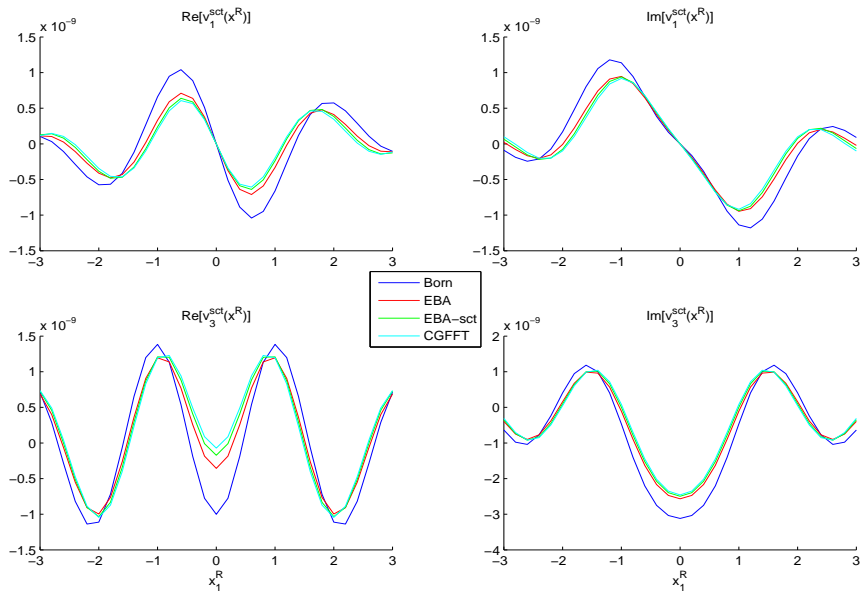


Fig. 17. The scattered field comparison among the four methods with frequency 0.5kHz: example III.

conditioners to increase the convergence rate of the linear equation solvers. With this CG-FFT method the stiffness matrix does not need to be stored, so that the memory storage is minimized.

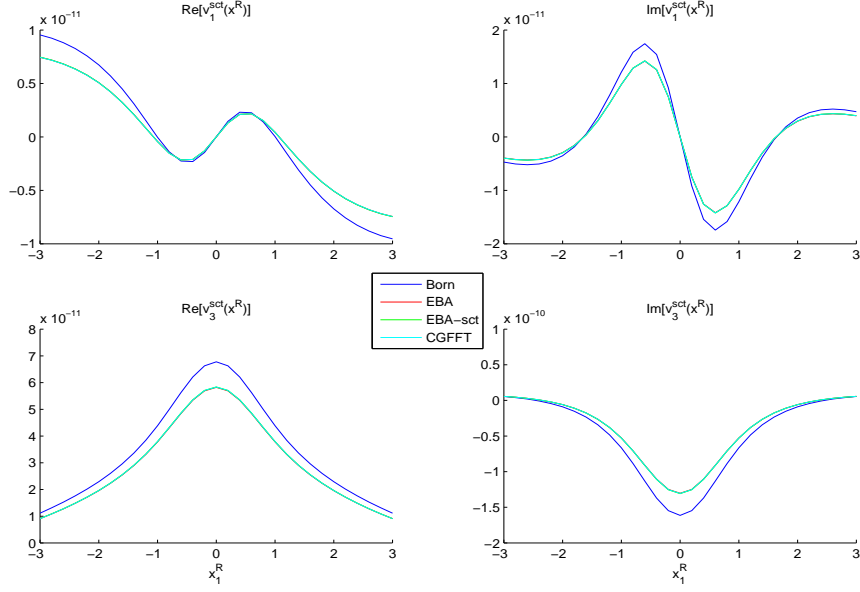


Fig. 18. The scattered field comparison among the four methods with frequency 0.5kHz: example III.

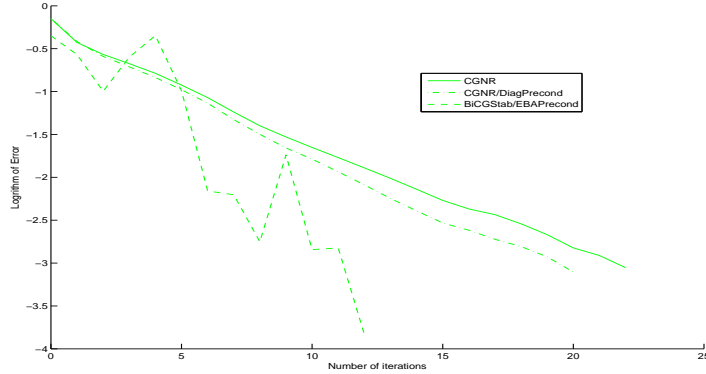


Fig. 19. The scattered field comparison among the three linear solvers with frequency 1.5kHz: example III.

## A Discretized Field Integral Equation

Following the discretization procedure, the complete discretized linear equation derived from Eq.(32)-Eq.(33) can be obtained. The discretized  $B_{p,q}^{\tau,\Lambda}$  are given by

$$B_{1,1}^{\tau,\Lambda} = \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^{\Lambda} (\tau_{1,1;m,n,l} + \tau_{2,2;m,n,l} + \tau_{3,3;m,n,l}) \quad (\text{A.1})$$

$$+ \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m,n,l}^{p,\Lambda} + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} (A_{m-1,n,l}^{p,\Lambda} - 2A_{m,n,l}^{p,\Lambda} + A_{m+1,n,l}^{p,\Lambda}), \quad (\text{A.2})$$

$$B_{2,2;m,n,l}^{\tau,\Lambda} = \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^\Lambda (\tau_{1,1;m,n,l} + \tau_{2,2;m,n,l} + \tau_{3,3;m,n,l}) \quad (\text{A.3})$$

$$+ \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m,n,l}^{p,\Lambda} + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_2)^2} (A_{m,n-1,l}^{p,\Lambda} - 2A_{m,n,l}^{p,\Lambda} + A_{m,n+1,l}^{p,\Lambda}), \quad (\text{A.4})$$

$$B_{3,3;m,n,l}^{\tau,\Lambda} = \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^\Lambda (\tau_{1,1;m,n,l} + \tau_{2,2;m,n,l} + \tau_{3,3;m,n,l}) \quad (\text{A.5})$$

$$+ \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m,n,l}^{p,\Lambda} + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_3)^2} (A_{m,n,l-1}^{p,\Lambda} - 2A_{m,n,l}^{p,\Lambda} + A_{m,n,l+1}^{p,\Lambda}), \quad (\text{A.6})$$

$$B_{1,2;m,n,l}^{\tau,\Lambda} = \frac{\lambda}{\rho c_p^2} \frac{1}{4\Delta x_1 \Delta x_2} (A_{m-1,n-1,l}^{p,\Lambda} - A_{m-1,n+1,l}^{p,\Lambda} - A_{m+1,n-1,l}^{p,\Lambda} + A_{m+1,n+1,l}^{p,\Lambda}), \quad (\text{A.7})$$

$$B_{1,3;m,n,l}^{\tau,\Lambda} = \frac{\lambda}{\rho c_p^2} \frac{1}{4\Delta x_1 \Delta x_3} (A_{m-1,n,l-1}^{p,\Lambda} - A_{m-1,n,l+1}^{p,\Lambda} - A_{m+1,n,l-1}^{p,\Lambda} + A_{m+1,n,l+1}^{p,\Lambda}), \quad (\text{A.8})$$

and

$$B_{2,3;m,n,l}^{\tau,\Lambda} = \frac{\lambda}{\rho c_p^2} \frac{1}{4\Delta x_2 \Delta x_3} (A_{m,n-1,l-1}^{p,\Lambda} - A_{m,n+1,l-1}^{p,\Lambda} - A_{m,n-1,l+1}^{p,\Lambda} + A_{m,n+1,l+1}^{p,\Lambda}). \quad (\text{A.9})$$

The discretized  $B_{p,q;m,n,l}^{\tau,M}$  are given by

$$B_{1,1;m,n,l}^{\tau,M} = -\chi_{m,n,l}^M \tau_{1,1;m,n,l} - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M (\tau_{1,1;m,n,l} + \tau_{2,2;m,n,l} + \tau_{3,3;m,n,l}) \quad (\text{A.10})$$

$$- \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m,n,l}^{p,M} - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} (A_{m-1,n,l}^{p,M} - 2A_{m,n,l}^{p,M} + A_{m+1,n,l}^{p,M})$$

$$\begin{aligned}
& -\frac{2}{(\Delta x_1)^2} (A_{1,1;m-1,n,l}^{s,M} - 2A_{1,1;m,n,l}^{s,M} + A_{1,1;m+1,n,l}^{s,M}) \\
& -\frac{1}{2\Delta x_1 \Delta x_2} (A_{1,2;m-1,n-1,l}^{s,M} - A_{1,2;m-1,n+1,l}^{s,M} - A_{1,2;m+1,n-1,l}^{s,M} + A_{1,2;m+1,n+1,l}^{s,M}) \\
& -\frac{1}{2\Delta x_1 \Delta x_3} (A_{1,3;m-1,n,l-1}^{s,M} - A_{1,3;m-1,n,l+1}^{s,M} - A_{1,3;m+1,n,l-1}^{s,M} + A_{1,3;m+1,n,l+1}^{s,M}) \\
& -\frac{\lambda}{\rho c_p^2} C_{m,n,l}^{p,M} \\
& -\frac{2c_s^2}{s^2} \frac{1}{(\Delta x_1)^2} \left[ (C_{m-1,n,l}^{p,M} - C_{m-1,n,l}^{s,M}) - 2(C_{m,n,l}^{p,M} - C_{m,n,l}^{s,M}) + (C_{m+1,n,l}^{p,M} - C_{m+1,n,l}^{s,M}) \right],
\end{aligned} \tag{A.11}$$

$$\begin{aligned}
B_{2,2;m,n,l}^{\tau,M} &= -\chi_{m,n,l}^M \tau_{2,2;m,n,l} - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M (\tau_{1,1;m,n,l} + \tau_{2,2;m,n,l} + \tau_{3,3;m,n,l}) \\
& -\frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m,n,l}^{p,M} - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_2)^2} (A_{m,n-1,l}^{p,M} - 2A_{m,n,l}^{p,M} + A_{m,n+1,l}^{p,M}) \\
& -\frac{1}{2\Delta x_1 \Delta x_2} (A_{1,2;m-1,n-1,l}^{s,M} - A_{1,2;m-1,n+1,l}^{s,M} - A_{1,2;m+1,n-1,l}^{s,M} + A_{1,2;m+1,n+1,l}^{s,M}) \\
& -\frac{2}{(\Delta x_2)^2} (A_{2,2;m,n-1,l}^{s,M} - 2A_{2,2;m,n,l}^{s,M} + A_{2,2;m,n+1,l}^{s,M}) \\
& -\frac{1}{2\Delta x_2 \Delta x_3} (A_{2,3;m,n-1,l-1}^{s,M} - A_{2,3;m,n-1,l+1}^{s,M} - A_{2,3;m,n+1,l-1}^{s,M} + A_{2,3;m,n+1,l+1}^{s,M}) \\
& -\frac{\lambda}{\rho c_p^2} C_{m,n,l}^{p,M} \\
& -\frac{2c_s^2}{s^2} \frac{1}{(\Delta x_2)^2} \left[ (C_{m,n-1,l}^{p,M} - C_{m,n-1,l}^{s,M}) - 2(C_{m,n,l}^{p,M} - C_{m,n,l}^{s,M}) + (C_{m,n+1,l}^{p,M} - C_{m,n+1,l}^{s,M}) \right],
\end{aligned} \tag{A.12}$$

$$\begin{aligned}
B_{3,3;m,n,l}^{\tau,M} &= -\chi_{m,n,l}^M \tau_{3,3;m,n,l} - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M (\tau_{1,1;m,n,l} + \tau_{2,2;m,n,l} + \tau_{3,3;m,n,l}) \\
& -\frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} A_{m,n,l}^{p,M} - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_3)^2} (A_{m,n,l-1}^{p,M} - 2A_{m,n,l}^{p,M} + A_{m,n,l+1}^{p,M}) \\
& -\frac{1}{2\Delta x_1 \Delta x_3} (A_{1,3;m-1,n,l-1}^{s,M} - A_{1,3;m-1,n,l+1}^{s,M} - A_{1,3;m+1,n,l-1}^{s,M} + A_{1,3;m+1,n,l+1}^{s,M}) \\
& -\frac{1}{2\Delta x_2 \Delta x_3} (A_{2,3;m,n-1,l-1}^{s,M} - A_{2,3;m,n-1,l+1}^{s,M} - A_{2,3;m,n+1,l-1}^{s,M} + A_{2,3;m,n+1,l+1}^{s,M}) \\
& -\frac{2}{(\Delta x_3)^2} (A_{3,3;m,n,l-1}^{s,M} - 2A_{3,3;m,n,l}^{s,M} + A_{3,3;m,n,l+1}^{s,M})
\end{aligned}$$

$$\begin{aligned}
& - \frac{\lambda}{\rho c_p^2} C_{m,n,l}^{p,M} \\
& - \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_3)^2} \left[ (C_{m,n,l-1}^{p,M} - C_{m,n,l-1}^{s,M}) - 2(C_{m,n,l}^{p,M} - C_{m,n,l}^{s,M}) + (C_{m,n,l+1}^{p,M} - C_{m,n,l+1}^{s,M}) \right],
\end{aligned} \tag{A.13}$$

$$\begin{aligned}
B_{1,2;m,n,l}^{\tau,M} &= -\chi_{m,n,l}^M \tau_{1,2;m,n,l} \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{4\Delta x_1 \Delta x_2} (A_{m-1,n-1,l}^{p,M} - A_{m-1,n+1,l}^{p,M} - A_{m+1,n-1,l}^{p,M} + A_{m+1,n+1,l}^{p,M}) \\
& - \frac{1}{(\Delta x_1)^2} (A_{1,2;m-1,n,l}^{s,M} - 2A_{1,2;m,n,l}^{s,M} + A_{1,2;m+1,n,l}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_2} (A_{1,1;m-1,n-1,l}^{s,M} - A_{1,1;m-1,n+1,l}^{s,M} - A_{1,1;m+1,n-1,l}^{s,M} + A_{1,1;m+1,n+1,l}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_2} (A_{2,2;m-1,n-1,l}^{s,M} - A_{2,2;m-1,n+1,l}^{s,M} - A_{2,2;m+1,n-1,l}^{s,M} + A_{2,2;m+1,n+1,l}^{s,M}) \\
& - \frac{1}{(\Delta x_2)^2} (A_{1,2;m,n-1,l}^{s,M} - 2A_{1,2;m,n,l}^{s,M} + A_{1,2;m,n+1,l}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_3} (A_{2,3;m-1,n,l-1}^{s,M} - A_{2,3;m-1,n,l+1}^{s,M} - A_{2,3;m+1,n,l-1}^{s,M} + A_{2,3;m+1,n,l+1}^{s,M}) \\
& - \frac{1}{4\Delta x_2 \Delta x_3} (A_{1,3;m,n-1,l-1}^{s,M} - A_{1,3;m,n-1,l+1}^{s,M} - A_{1,3;m,n+1,l-1}^{s,M} + A_{1,3;m,n+1,l+1}^{s,M}) \\
& - \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_1 \Delta x_2} \left[ (C_{m-1,n-1,l}^{p,M} - C_{m-1,n-1,l}^{s,M}) - (C_{m-1,n+1,l}^{p,M} - C_{m-1,n+1,l}^{s,M}) \right. \\
& \left. - (C_{m+1,n-1,l}^{p,M} - C_{m+1,n-1,l}^{s,M}) + (C_{m+1,n+1,l}^{p,M} - C_{m+1,n+1,l}^{s,M}) \right],
\end{aligned} \tag{A.14}$$

$$\begin{aligned}
B_{1,3;m,n,l}^{\tau,M} &= -\chi_{m,n,l}^M \tau_{1,3;m,n,l} \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{4\Delta x_1 \Delta x_3} (A_{m-1,n,l-1}^{p,M} - A_{m-1,n,l+1}^{p,M} - A_{m+1,n,l-1}^{p,M} + A_{m+1,n,l+1}^{p,M}) \\
& - \frac{1}{(\Delta x_1)^2} (A_{1,3;m-1,n,l}^{s,M} - 2A_{1,3;m,n,l}^{s,M} + A_{1,3;m+1,n,l}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_3} (A_{1,1;m-1,n,l-1}^{s,M} - A_{1,1;m-1,n,l+1}^{s,M} - A_{1,1;m+1,n,l-1}^{s,M} + A_{1,1;m+1,n,l+1}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_2} (A_{2,3;m-1,n-1,l}^{s,M} - A_{2,3;m-1,n+1,l}^{s,M} - A_{2,3;m+1,n-1,l}^{s,M} + A_{2,3;m+1,n+1,l}^{s,M}) \\
& - \frac{1}{4\Delta x_2 \Delta x_3} (A_{1,2;m,n-1,l-1}^{s,M} - A_{1,2;m,n-1,l+1}^{s,M} - A_{1,2;m,n+1,l-1}^{s,M} + A_{1,2;m,n+1,l+1}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_3} (A_{3,3;m-1,n,l-1}^{s,M} - A_{3,3;m-1,n,l+1}^{s,M} - A_{3,3;m+1,n,l-1}^{s,M} + A_{3,3;m+1,n,l+1}^{s,M})
\end{aligned}$$

$$\begin{aligned}
& - \frac{1}{(\Delta x_3)^2} (A_{1,3;m,n,l-1}^{s,M} - 2A_{1,3;m,n,l}^{s,M} + A_{1,3;m,n,l+1}^{s,M}) \\
& - \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_1 \Delta x_3} \left[ (C_{m-1,n,l-1}^{p,M} - C_{m-1,n,l-1}^{s,M}) - (C_{m-1,n,l+1}^{p,M} - C_{m-1,n,l+1}^{s,M}) \right. \\
& \left. - (C_{m+1,n,l-1}^{p,M} - C_{m+1,n,l-1}^{s,M}) + (C_{m+1,n,l+1}^{p,M} - C_{m+1,n,l+1}^{s,M}) \right], \tag{A.15}
\end{aligned}$$

and

$$\begin{aligned}
B_{2,3;m,n,l}^{\tau,M} &= -\chi_{m,n,l}^{\tau,2,3;m,n,l} \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{4\Delta x_2 \Delta x_3} (A_{m,n-1,l-1}^{p,M} - A_{m,n-1,l+1}^{p,M} - A_{m,n+1,l-1}^{p,M} + A_{m,n+1,l+1}^{p,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_2} (A_{1,3;m-1,n-1,l}^{s,M} - A_{1,3;m-1,n+1,l}^{s,M} - A_{1,3;m+1,n-1,l}^{s,M} + A_{1,3;m+1,n+1,l}^{s,M}) \\
& - \frac{1}{4\Delta x_1 \Delta x_3} (A_{1,2;m-1,n,l-1}^{s,M} - A_{1,2;m-1,n,l+1}^{s,M} - A_{1,2;m+1,n,l-1}^{s,M} + A_{1,2;m+1,n,l+1}^{s,M}) \\
& - \frac{1}{(\Delta x_2)^2} (A_{2,3;m,n-1,l}^{s,M} - 2A_{2,3;m,n,l}^{s,M} + A_{2,3;m,n+1,l}^{s,M}) \\
& - \frac{1}{4\Delta x_2 \Delta x_3} (A_{2,2;m,n-1,l-1}^{s,M} - A_{2,2;m,n-1,l+1}^{s,M} - A_{2,2;m,n+1,l-1}^{s,M} + A_{2,2;m,n+1,l+1}^{s,M}) \\
& - \frac{1}{4\Delta x_2 \Delta x_3} (A_{3,3;m,n-1,l-1}^{s,M} - A_{3,3;m,n-1,l+1}^{s,M} - A_{3,3;m,n+1,l-1}^{s,M} + A_{3,3;m,n+1,l+1}^{s,M}) \\
& - \frac{1}{(\Delta x_3)^2} (A_{2,3;m,n,l-1}^{s,M} - 2A_{2,3;m,n,l}^{s,M} + A_{2,3;m,n,l+1}^{s,M}) \\
& - \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_2 \Delta x_3} \left[ (C_{m,n-1,l-1}^{p,M} - C_{m,n-1,l-1}^{s,M}) - (C_{m,n-1,l+1}^{p,M} - C_{m,n-1,l+1}^{s,M}) \right. \\
& \left. - (C_{m,n+1,l-1}^{p,M} - C_{m,n+1,l-1}^{s,M}) + (C_{m,n+1,l+1}^{p,M} - C_{m,n+1,l+1}^{s,M}) \right]. \tag{A.16}
\end{aligned}$$

The discretized  $B_{p,q;m,n,l}^{\tau,\rho}$  are given by

$$\begin{aligned}
B_{1,1;m,n,l}^{\tau,\rho} &= -\frac{\lambda}{\rho c_p^2} \frac{s}{c_s} D_{m,n,l}^{p,\rho} \\
& - \frac{2s}{c_s} \frac{1}{2\Delta x_1} (A_{1;m+1,n,l}^{s,\rho} - A_{1;m-1,n,l}^{s,\rho}) \\
& - \frac{2u}{s\rho c_s} \frac{1}{(\Delta x_1)^2} \left[ (D_{m-1,n,l}^{p,\rho} - D_{m-1,n,l}^{s,\rho}) - 2(D_{m,n,l}^{p,\rho} - D_{m,n,l}^{s,\rho}) + (D_{m+1,n,l}^{p,\rho} - D_{m+1,n,l}^{s,\rho}) \right], \tag{A.17}
\end{aligned}$$

$$\begin{aligned}
B_{2,2;m,n,l}^{\tau,\rho} &= -\frac{\lambda}{\rho c_p^2} \frac{s}{c_s} D_{m,n,l}^{\text{p},\rho} \\
&- \frac{2s}{c_s} \frac{1}{2\Delta x_2} (A_{2;m,n+1,l}^{\text{s},\rho} - A_{2;m,n-1,l}^{\text{s},\rho}) \\
&- \frac{2u}{s\rho c_s} \frac{1}{(\Delta x_2)^2} \left[ (D_{m,n-1,l}^{\text{p},\rho} - D_{m,n-1,l}^{\text{s},\rho}) - 2(D_{m,n,l}^{\text{p},\rho} - D_{m,n,l}^{\text{s},\rho}) + (D_{m,n+1,l}^{\text{p},\rho} - D_{m,n+1,l}^{\text{s},\rho}) \right],
\end{aligned} \tag{A.18}$$

$$\begin{aligned}
B_{3,3;m,n,l}^{\tau,\rho} &= -\frac{\lambda}{\rho c_p^2} \frac{s}{c_s} D_{m,n,l}^{\text{p},\rho} \\
&- \frac{2s}{c_s} \frac{1}{2\Delta x_3} (A_{3;m,n,l+1}^{\text{s},\rho} - A_{3;m,n,l-1}^{\text{s},\rho}) \\
&- \frac{2u}{s\rho c_s} \frac{1}{(\Delta x_3)^2} \left[ (D_{m,n,l-1}^{\text{p},\rho} - D_{m,n,l-1}^{\text{s},\rho}) - 2(D_{m,n,l}^{\text{p},\rho} - D_{m,n,l}^{\text{s},\rho}) + (D_{m,n,l+1}^{\text{p},\rho} - D_{m,n,l+1}^{\text{s},\rho}) \right],
\end{aligned} \tag{A.19}$$

$$\begin{aligned}
B_{1,2;m,n,l}^{\tau,\rho} &= -\frac{s}{c_s} \frac{1}{2\Delta x_1} (A_{2;m+1,n,l}^{\text{s},\rho} - A_{2;m-1,n,l}^{\text{s},\rho}) \\
&- \frac{s}{c_s} \frac{1}{2\Delta x_2} (A_{1;m,n+1,l}^{\text{s},\rho} - A_{1;m,n-1,l}^{\text{s},\rho}) \\
&- \frac{2u}{s\rho c_s} \frac{1}{4\Delta x_1 \Delta x_2} \left[ (D_{m-1,n-1,l}^{\text{p},\rho} - D_{m-1,n-1,l}^{\text{s},\rho}) - (D_{m-1,n+1,l}^{\text{p},\rho} - D_{m-1,n+1,l}^{\text{s},\rho}) \right. \\
&- \left. (D_{m+1,n-1,l}^{\text{p},\rho} - D_{m+1,n-1,l}^{\text{s},\rho}) + (D_{m+1,n+1,l}^{\text{p},\rho} - D_{m+1,n+1,l}^{\text{s},\rho}) \right],
\end{aligned} \tag{A.20}$$

$$\begin{aligned}
B_{1,3;m,n,l}^{\tau,\rho} &= -\frac{s}{c_s} \frac{1}{2\Delta x_1} (A_{3;m+1,n,l}^{\text{s},\rho} - A_{3;m-1,n,l}^{\text{s},\rho}) \\
&- \frac{s}{c_s} \frac{1}{2\Delta x_3} (A_{1;m,n,l+1}^{\text{s},\rho} - A_{1;m,n,l-1}^{\text{s},\rho}) \\
&- \frac{2u}{s\rho c_s} \frac{1}{4\Delta x_1 \Delta x_3} \left[ (D_{m-1,n,l-1}^{\text{p},\rho} - D_{m-1,n,l-1}^{\text{s},\rho}) - (D_{m-1,n,l+1}^{\text{p},\rho} - D_{m-1,n,l+1}^{\text{s},\rho}) \right. \\
&- \left. (D_{m+1,n,l-1}^{\text{p},\rho} - D_{m+1,n,l-1}^{\text{s},\rho}) + (D_{m+1,n,l+1}^{\text{p},\rho} - D_{m+1,n,l+1}^{\text{s},\rho}) \right],
\end{aligned} \tag{A.21}$$

and

$$B_{2,3;m,n,l}^{\tau,\rho} = -\frac{s}{c_s} \frac{1}{2\Delta x_2} (A_{3;m,n+1,l}^{\text{s},\rho} - A_{3;m,n-1,l}^{\text{s},\rho})$$

$$\begin{aligned}
& - \frac{s}{c_s} \frac{1}{2\Delta x_3} (A_{2;m,n,l+1}^{s,\rho} - A_{2;m,n,l-1}^{s,\rho}) \\
& - \frac{2u}{s\rho c_s} \frac{1}{4\Delta x_2 \Delta x_3} \left[ (D_{m,n-1,l-1}^{p,\rho} - D_{m,n-1,l-1}^{s,\rho}) - (D_{m,n-1,l+1}^{p,\rho} - D_{m,n-1,l+1}^{s,\rho}) \right. \\
& \left. - (D_{m,n+1,l-1}^{p,\rho} - D_{m,n+1,l-1}^{s,\rho}) + (D_{m,n+1,l+1}^{p,\rho} - D_{m,n+1,l+1}^{s,\rho}) \right].
\end{aligned} \tag{A.22}$$

The discretized  $B_{r;m,n,l}^{u,\Lambda}$  are given by

$$B_{1;m,n,l}^{u,\Lambda} = -\frac{\lambda s c_s}{2\mu c_p^2} \frac{1}{2\Delta x_1} (A_{m+1,n,l}^{p,\Lambda} - A_{m-1,n,l}^{p,\Lambda}), \tag{A.23}$$

$$B_{2;m,n,l}^{u,\Lambda} = -\frac{\lambda s c_s}{2\mu c_p^2} \frac{1}{2\Delta x_2} (A_{m,n+1,l}^{p,\Lambda} - A_{m,n-1,l}^{p,\Lambda}), \tag{A.24}$$

and

$$B_{3;m,n,l}^{u,\Lambda} = -\frac{\lambda s c_s}{2\mu c_p^2} \frac{1}{2\Delta x_3} (A_{m,n,l+1}^{p,\Lambda} - A_{m,n,l-1}^{p,\Lambda}). \tag{A.25}$$

The discretized  $B_{r;m,n,l}^{u,M}$  are given by

$$\begin{aligned}
B_{1;m,n,l}^{u,M} &= \frac{\lambda s c_s}{2\mu c_p^2} \frac{1}{2\Delta x_1} (A_{m+1,n,l}^{p,M} - A_{m-1,n,l}^{p,M}) \\
&+ \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_1} (A_{1,1;m+1,n,l}^{s,M} - A_{1,1;m-1,n,l}^{s,M}) \\
&+ \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_2} (A_{1,2;m,n+1,l}^{s,M} - A_{1,2;m,n-1,l}^{s,M}) \\
&+ \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_3} (A_{1,3;m,n,l+1}^{s,M} - A_{1,3;m,n,l-1}^{s,M}) \\
&+ \frac{c_s}{s} \frac{1}{2\Delta x_1} \left[ (C_{m+1,n,l}^{p,M} - C_{m+1,n,l}^{s,M}) - (C_{m-1,n,l}^{p,M} - C_{m-1,n,l}^{s,M}) \right],
\end{aligned} \tag{A.27}$$

$$\begin{aligned}
B_{2;m,n,l}^{u,M} &= \frac{\lambda s c_s}{2\mu c_p^2} \frac{1}{2\Delta x_2} (A_{m,n+1,l}^{p,M} - A_{m,n-1,l}^{p,M}) \\
&+ \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_1} (A_{1,2;m+1,n,l}^{s,M} - A_{1,2;m-1,n,l}^{s,M})
\end{aligned} \tag{A.28}$$

$$\begin{aligned}
& + \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_2} (A_{2,2;m,n+1,l}^{s,M} - A_{2,2;m,n-1,l}^{s,M}) \\
& + \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_3} (A_{2,3;m,n,l+1}^{s,M} - A_{2,3;m,n,l-1}^{s,M}) \\
& + \frac{c_s}{s} \frac{1}{2\Delta x_2} [(C_{m,n+1,l}^{p,M} - C_{m,n+1,l}^{s,M}) - (C_{m,n-1,l}^{p,M} - C_{m,n-1,l}^{s,M})] , \tag{A.29}
\end{aligned}$$

and

$$\begin{aligned}
B_{3;m,n,l}^{u,M} & = \frac{\lambda s c_s}{2\mu c_p^2} \frac{1}{2\Delta x_3} (A_{m,n,l+1}^{p,M} - A_{m,n,l-1}^{p,M}) \tag{A.30} \\
& + \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_1} (A_{1,3;m+1,n,l}^{s,M} - A_{1,3;m-1,n,l}^{s,M}) \\
& + \frac{s}{\mu} \frac{1}{2\Delta x_2} (A_{2,3;m,n+1,l}^{s\rho c_s,M} - A_{2,3;m,n-1,l}^{s,M}) \\
& + \frac{s\rho c_s}{\mu} \frac{1}{2\Delta x_3} (A_{3,3;m,n,l+1}^{s,M} - A_{3,3;m,n,l-1}^{s,M}) \\
& + \frac{c_s}{s} \frac{1}{2\Delta x_3} [(C_{m,n,l+1}^{p,M} - C_{m,n,l+1}^{s,M}) - (C_{m,n,l-1}^{p,M} - C_{m,n,l-1}^{s,M})] . \tag{A.31}
\end{aligned}$$

The discretized  $B_{r;m,n,l}^{u,\rho}$  are given by

$$\begin{aligned}
B_{1;m,n,l}^{u,\rho} & = \frac{s^2}{c_s^2} A_{1;m,n,l}^{s,\rho} \tag{A.32} \\
& + \frac{1}{(\Delta x_1)^2} [(A_{1;m-1,n,l}^{p,\rho} - A_{1;m-1,n,l}^{s,\rho}) - 2(A_{1;m,n,l}^{p,\rho} - A_{1;m,n,l}^{s,\rho}) + (A_{1;m+1,n,l}^{p,\rho} - A_{1;m+1,n,l}^{s,\rho})] \\
& + \frac{1}{4\Delta x_1 \Delta x_2} [(A_{2;m-1,n-1,l}^{p,\rho} - A_{2;m-1,n-1,l}^{s,\rho}) - (A_{2;m-1,n+1,l}^{p,\rho} - A_{2;m-1,n+1,l}^{s,\rho}) \\
& - (A_{2;m+1,n-1,l}^{p,\rho} - A_{2;m+1,n-1,l}^{s,\rho}) + (A_{2;m+1,n+1,l}^{p,\rho} - A_{2;m+1,n+1,l}^{s,\rho})] \\
& + \frac{1}{4\Delta x_1 \Delta x_3} [(A_{3;m-1,n,l-1}^{p,\rho} - A_{3;m-1,n,l-1}^{s,\rho}) - (A_{3;m-1,n,l+1}^{p,\rho} - A_{3;m-1,n,l+1}^{s,\rho}) \\
& - (A_{3;m+1,n,l-1}^{p,\rho} - A_{3;m+1,n,l-1}^{s,\rho}) + (A_{3;m+1,n,l+1}^{p,\rho} - A_{3;m+1,n,l+1}^{s,\rho})] , \tag{A.33}
\end{aligned}$$

$$\begin{aligned}
B_{2;m,n,l}^{u,\rho} & = \frac{s^2}{c_s^2} A_{2;m,n,l}^{s,\rho} \tag{A.34} \\
& + \frac{1}{4\Delta x_1 \Delta x_2} [(A_{1;m-1,n-1,l}^{p,\rho} - A_{1;m-1,n-1,l}^{s,\rho}) - (A_{1;m-1,n+1,l}^{p,\rho} - A_{1;m-1,n+1,l}^{s,\rho}) \\
& - (A_{1;m+1,n-1,l}^{p,\rho} - A_{1;m+1,n-1,l}^{s,\rho}) + (A_{1;m+1,n+1,l}^{p,\rho} - A_{1;m+1,n+1,l}^{s,\rho})]
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{(\Delta x_2)^2} \left[ (A_{2;m,n-1,l}^{\text{p},\rho} - A_{2;m,n-1,l}^{\text{s},\rho}) - 2(A_{2;m,n,l}^{\text{p},\rho} - A_{2;m,n,l}^{\text{s},\rho}) + (A_{2;m,n+1,l}^{\text{p},\rho} - A_{2;m,n+1,l}^{\text{s},\rho}) \right] \\
& + \frac{1}{4\Delta x_2 \Delta x_3} \left[ (A_{3;m,n-1,l-1}^{\text{p},\rho} - A_{3;m,n-1,l-1}^{\text{s},\rho}) - (A_{3;m,n-1,l+1}^{\text{p},\rho} - A_{3;m,n-1,l+1}^{\text{s},\rho}) \right. \\
& \left. - (A_{3;m,n+1,l-1}^{\text{p},\rho} - A_{3;m,n+1,l-1}^{\text{s},\rho}) + (A_{3;m,n+1,l+1}^{\text{p},\rho} - A_{3;m,n+1,l+1}^{\text{s},\rho}) \right], \tag{A.35}
\end{aligned}$$

and

$$\begin{aligned}
B_{3;m,n,l}^{u,\rho} & = \frac{s^2}{c_s^2} A_{3;m,n,l}^{\text{s},\rho} \tag{A.36} \\
& + \frac{1}{4\Delta x_1 \Delta x_3} \left[ (A_{1;m-1,n,l-1}^{\text{p},\rho} - A_{1;m-1,n,l-1}^{\text{s},\rho}) - (A_{1;m-1,n,l+1}^{\text{p},\rho} - A_{1;m-1,n,l+1}^{\text{s},\rho}) \right. \\
& \left. - (A_{1;m+1,n,l-1}^{\text{p},\rho} - A_{1;m+1,n,l-1}^{\text{s},\rho}) + (A_{1;m+1,n,l+1}^{\text{p},\rho} - A_{1;m+1,n,l+1}^{\text{s},\rho}) \right] \\
& + \frac{1}{4\Delta x_2 \Delta x_3} \left[ (A_{2;m,n-1,l-1}^{\text{p},\rho} - A_{2;m,n-1,l-1}^{\text{s},\rho}) - (A_{2;m,n-1,l+1}^{\text{p},\rho} - A_{2;m,n-1,l+1}^{\text{s},\rho}) \right. \\
& \left. - (A_{2;m,n+1,l-1}^{\text{p},\rho} - A_{2;m,n+1,l-1}^{\text{s},\rho}) + (A_{2;m,n+1,l+1}^{\text{p},\rho} - A_{2;m,n+1,l+1}^{\text{s},\rho}) \right] \\
& + \frac{1}{(\Delta x_3)^2} \left[ (A_{3;m,n,l-1}^{\text{p},\rho} - A_{3;m,n,l-1}^{\text{s},\rho}) - 2(A_{3;m,n,l}^{\text{p},\rho} - A_{3;m,n,l}^{\text{s},\rho}) + (A_{3;m,n,l+1}^{\text{p},\rho} - A_{3;m,n,l+1}^{\text{s},\rho}) \right]. \tag{A.37}
\end{aligned}$$

In addition, let  $\gamma \in \{\text{p}, \text{s}\}$  and  $\beta \in \{\Lambda, M\}$ , those  $A_{i,j;m,n,l}^{\gamma,\beta}$  and  $A_{r;m,n,l}^{\gamma,\rho}$  are defined by

$$\begin{aligned}
A_{i,j;m,n,l}^{\gamma,\beta} & = A_{i,j}^{\gamma,\beta}(x_1; m, x_2; n, x_3; l) = \\
& \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \mathcal{G}_{m-m', n-n', l-l'}^{\gamma} \chi_{m', n', l'}^{\beta} \tau_{i,j; m', n', l'}, \tag{A.38}
\end{aligned}$$

and

$$\begin{aligned}
A_{r;m,n,l}^{\gamma,\rho} & = A_r^{\gamma,\rho}(x_1; m, x_2; n, x_3; l) = \\
& \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=1}^M \sum_{n'=1}^N \sum_{l'=1}^L \mathcal{G}_{m-m', n-n', l-l'}^{\gamma} \chi_{m', n', l'}^{\rho} u_{r; m', n', l'}, \tag{A.39}
\end{aligned}$$

for  $m = -1, \dots, M+2$ ,  $n = -1, \dots, N+2$ , and  $l = -1, \dots, L+2$ , where  $A_{k,k;m,n,l}^{\gamma,\beta}$  is abbreviated by  $A_{m,n,l}^{\gamma,\beta}$ .

Those  $C_{m,n,l}^{\gamma,\beta}$  and  $D_{m,n,l}^{\gamma,\rho}$  are defined by

$$C_{m,n,l}^{\gamma,\beta} = \left( \partial_i \partial_j A_{i,j}^{\gamma,\beta} \right)_{m,n,l} \quad (\text{A.40})$$

$$\begin{aligned}
&= \frac{1}{(\Delta x_1)^2} (A_{1,1;m-1,n,l}^{\gamma,\beta} - 2A_{1,1;m,n,l}^{\gamma,\beta} + A_{1,1;m+1,n,l}^{\gamma,\beta}) \\
&+ \frac{1}{(\Delta x_2)^2} (A_{2,2;m,n-1,l}^{\gamma,\beta} - 2A_{2,2;m,n,l}^{\gamma,\beta} + A_{2,2;m,n+1,l}^{\gamma,\beta}) \\
&+ \frac{1}{(\Delta x_3)^2} (A_{3,3;m,n,l-1}^{\gamma,\beta} - 2A_{3,3;m,n,l}^{\gamma,\beta} + A_{3,3;m,n,l+1}^{\gamma,\beta}) \\
&+ \frac{1}{2\Delta x_1 \Delta x_2} (A_{1,2;m-1,n-1,l}^{\gamma,\beta} - A_{1,2;m-1,n+1,l}^{\gamma,\beta} - A_{1,2;m+1,n-1,l}^{\gamma,\beta} + A_{1,2;m+1,n+1,l}^{\gamma,\beta}) \\
&+ \frac{1}{2\Delta x_1 \Delta x_3} (A_{1,3;m-1,n,l-1}^{\gamma,\beta} - A_{1,3;m-1,n,l+1}^{\gamma,\beta} - A_{1,3;m+1,n,l-1}^{\gamma,\beta} + A_{1,3;m+1,n,l+1}^{\gamma,\beta}) \\
&+ \frac{1}{2\Delta x_2 \Delta x_3} (A_{2,3;m,n-1,l-1}^{\gamma,\beta} - A_{2,3;m,n-1,l+1}^{\gamma,\beta} - A_{2,3;m,n+1,l-1}^{\gamma,\beta} + A_{2,3;m,n+1,l+1}^{\gamma,\beta}),
\end{aligned} \quad (\text{A.41})$$

$$D_{m,n,l}^{\gamma,\rho} = (\partial_k A_k^{\gamma,\rho})_{m,n,l} \quad (\text{A.42})$$

$$\begin{aligned}
&= \frac{1}{2\Delta x_1} (A_{1;m+1,n,l}^{\gamma,\rho} - A_{1;m-1,n,l}^{\gamma,\rho}) + \frac{1}{2\Delta x_2} (A_{2;m,n+1,l}^{\gamma,\rho} - A_{2;m,n-1,l}^{\gamma,\rho}) \\
&+ \frac{1}{2\Delta x_3} (A_{3;m,n,l+1}^{\gamma,\rho} - A_{3;m,n,l-1}^{\gamma,\rho}),
\end{aligned} \quad (\text{A.43})$$

for  $m = 0, \dots, M+1$ ,  $n = 0, \dots, N+1$ , and  $l = 0, \dots, L+1$ .

## B Complete explicit expression of the adjoint operator

The adjoint operator  $\mathcal{K}^*$  is recognized as

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{1,1;m,n,l} &= \frac{\overline{\lambda}}{\rho c_p^2} \overline{\chi_{m,n,l}^\Lambda} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
&- \overline{\chi_{m,n,l}^M} r_{1,1;m,n,l} - \left( \frac{\overline{\lambda}}{\rho c_p^2} \right) \overline{\chi_{m,n,l}^M} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
&+ \overline{\chi_{m,n,l}^\Lambda} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{m',n',l'}^{\text{p},\Lambda} \\
&- \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{1,1;m',n',l'}^{\text{p},M}
\end{aligned}$$

$$\begin{aligned}
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{1,1;m',n',l'}^{s,M}, \\
& \hspace{15em} \text{(B.1)}
\end{aligned}$$

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{2,2;m,n,l} &= \frac{\overline{\lambda}}{\rho c_p^2} \overline{\chi_{m,n,l}^\Lambda} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
& - \overline{\chi_{m,n,l}^M} r_{2,2;m,n,l} - \left( \frac{\overline{\lambda}}{\rho c_p^2} \right) \overline{\chi_{m,n,l}^M} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
& + \overline{\chi_{m,n,l}^\Lambda} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{m',n',l'}^{p,\Lambda} \\
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{2,2;m',n',l'}^{p,M} \\
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{2,2;m',n',l'}^{s,M}, \\
& \hspace{15em} \text{(B.2)}
\end{aligned}$$

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{3,3;m,n,l} &= \frac{\overline{\lambda}}{\rho c_p^2} \overline{\chi_{m,n,l}^\Lambda} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
& - \overline{\chi_{m,n,l}^M} r_{3,3;m,n,l} - \left( \frac{\overline{\lambda}}{\rho c_p^2} \right) \overline{\chi_{m,n,l}^M} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
& + \overline{\chi_{m,n,l}^\Lambda} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{m',n',l'}^{p,\Lambda} \\
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{3,3;m',n',l'}^{p,M} \\
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{3,3;m',n',l'}^{s,M}, \\
& \hspace{15em} \text{(B.3)}
\end{aligned}$$

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{1,2;m,n,l} &= - \overline{\chi_{m,n,l}^M} r_{1,2;m,n,l} \\
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{1,2;m',n',l'}^{p,M} \\
& - \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{1,2;m',n',l'}^{s,M},
\end{aligned}$$

(B.4)

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{1,3;m,n,l} &= -\overline{\chi_{m,n,l}^M} r_{1,3;m,n,l} \\
&- \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{1,3;m',n',l'}^{\text{P},M} \\
&- \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{1,3;m',n',l'}^{\text{S},M},
\end{aligned} \tag{B.5}$$

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{2,3;m,n,l} &= -\overline{\chi_{m,n,l}^M} r_{2,3;m,n,l} \\
&- \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{2,3;m',n',l'}^{\text{P},M} \\
&- \overline{\chi_{m,n,l}^M} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{2,3;m',n',l'}^{\text{S},M},
\end{aligned} \tag{B.6}$$

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{0,1;m,n,l} &= -\overline{\chi_{m,n,l}^\rho} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{0,1;m',n',l'}^{\text{P},\rho} \\
&- \overline{\chi_{m,n,l}^\rho} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{0,1;m',n',l'}^{\text{S},\rho},
\end{aligned} \tag{B.7}$$

$$\begin{aligned}
(\mathcal{K}^* r_{p,q})_{0,2;m,n,l} &= -\overline{\chi_{m,n,l}^\rho} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{0,2;m',n',l'}^{\text{P},\rho} \\
&- \overline{\chi_{m,n,l}^\rho} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{0,2;m',n',l'}^{\text{S},\rho},
\end{aligned} \tag{B.8}$$

and

$$(\mathcal{K}^* r_{p,q})_{0,3;m,n,l} = -\overline{\chi_{m,n,l}^\rho} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^p}_{m'-m, n'-n, l'-l} F_{0,3;m',n',l'}^{\text{P},\rho}$$

$$-\overline{\chi_{m,n,l}^\rho} \Delta x_1 \Delta x_2 \Delta x_3 \sum_{m'=-1}^{M+2} \sum_{n'=-1}^{N+2} \sum_{l'=-1}^{L+2} \overline{\mathcal{G}^s}_{m'-m, n'-n, l'-l} F_{0,3;m',n',l'}^{\text{S},\rho}, \quad (\text{B.9})$$

for  $m = 1, \dots, M$ ,  $n = 1, \dots, N$ , and  $l = 1, \dots, L$ , where

$$\begin{aligned} F_{m,n,l}^{\text{P},\Lambda} = & \overline{\left( \frac{\lambda}{\rho c_p^2} \right)} \left[ \overline{\left( \frac{\lambda s^2}{2\mu c_p^2} \right)} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{2,2;m,n,l}) \right. \\ & + \frac{1}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\ & + \frac{1}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\ & + \frac{1}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{2,2;m,n,l} + r_{2,2;m,n,l+1}) \\ & + \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\ & + \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\ & + \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n+1,l-1} - r_{2,3;m,n-1,l+1} + r_{2,3;m,n+1,l+1}) \\ & - \overline{\left( \frac{s\rho c_s}{2\mu} \right)} \frac{1}{2\Delta x_1} (r_{1;m-1,n,l} - r_{1;m+1,n,l}) \\ & - \overline{\left( \frac{s\rho c_s}{2\mu} \right)} \frac{1}{2\Delta x_2} (r_{2;m,n-1,l} - r_{2;m,n+1,l}) \\ & \left. - \overline{\left( \frac{s\rho c_s}{2\mu} \right)} \frac{1}{2\Delta x_3} (r_{3;m,n,l-1} - r_{3;m,n,l+1}) \right], \quad (\text{B.10}) \end{aligned}$$

$$\begin{aligned} F_{1,1;m,n,l}^{\text{P},M} = & \overline{\left( \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \right)} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\ & + \overline{\left( \frac{2\lambda}{\rho c_p^2} \right)} \frac{1}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\ & + \overline{\left( \frac{\lambda}{\rho c_p^2} \right)} \frac{1}{(\Delta x_1)^2} (r_{2,2;m-1,n,l} - 2r_{2,2;m,n,l} + r_{2,2;m+1,n,l}) \\ & + \overline{\left( \frac{\lambda}{\rho c_p^2} \right)} \frac{1}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\ & + \overline{\left( \frac{\lambda}{\rho c_p^2} \right)} \frac{1}{(\Delta x_1)^2} (r_{3,3;m-1,n,l} - 2r_{3,3;m,n,l} + r_{3,3;m+1,n,l}) \end{aligned}$$

$$\begin{aligned}
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{3,3;m,n,l} + r_{3,3;m,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n+1,l-1} - r_{2,3;m,n-1,l+1} + r_{2,3;m,n+1,l+1}) \\
& + \overline{\left(\frac{2c_s^2}{s^2}\right)} \frac{1}{(\Delta x_1)^2} (t_{m-1,n,l} - 2t_{m,n,l} + t_{m+1,n,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_1} (r_{0,1;m-1,n,l} - r_{0,1;m+1,n,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_2} (r_{0,2;m,n-1,l} - r_{0,2;m,n+1,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_3} (r_{0,3;m,n,l-1} - r_{0,3;m,n,l+1}) \\
& - \overline{\left(\frac{c_s}{s}\right)} \frac{1}{(\Delta x_1)^2} (d_{m-1,n,l} - 2d_{m,n,l} + d_{m+1,n,l}), \tag{B.11}
\end{aligned}$$

$$\begin{aligned}
F_{2,2;m,n,l}^{\text{p},M} & = \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2}\right)} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_2)^2} (r_{1,1;m,n-1,l} - 2r_{1,1;m,n,l} + r_{1,1;m,n+1,l}) \\
& + \overline{\left(\frac{2\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_2)^2} (r_{3,3;m,n-1,l} - 2r_{3,3;m,n,l} + r_{3,3;m,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{3,3;m,n,l} + r_{3,3;m,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1})
\end{aligned}$$

$$\begin{aligned}
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n+1,l-1} - r_{2,3;m,n-1,l+1} + r_{2,3;m,n+1,l+1}) \\
& + \overline{\left(\frac{2c_s^2}{s^2}\right)} \frac{1}{(\Delta x_2)^2} (t_{m,n-1,l} - 2t_{m,n,l} + t_{m,n+1,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_1} (r_{0,1;m-1,n,l} - r_{0,1;m+1,n,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_2} (r_{0,2;m,n-1,l} - r_{0,2;m,n+1,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_3} (r_{0,3;m,n,l-1} - r_{0,3;m,n,l+1}) \\
& - \overline{\left(\frac{c_s}{s}\right)} \frac{1}{(\Delta x_2)^2} (d_{m,n-1,l} - 2d_{m,n,l} + d_{m,n+1,l}), \tag{B.12}
\end{aligned}$$

$$\begin{aligned}
F_{3,3;m,n,l}^{\text{P},M} & = \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2}\right)} (r_{1,1;m,n,l} + r_{2,2;m,n,l} + r_{3,3;m,n,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_3)^2} (r_{1,1;m,n,l-1} - 2r_{1,1;m,n,l} + r_{1,1;m,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_3)^2} (r_{2,2;m,n,l-1} - 2r_{2,2;m,n,l} + r_{2,2;m,n,l+1}) \\
& + \overline{\left(\frac{2\lambda}{\rho c_p^2}\right)} \frac{1}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{3,3;m,n,l} + r_{3,3;m,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n+1,l-1} - r_{2,3;m,n-1,l+1} + r_{2,3;m,n+1,l+1}) \\
& + \overline{\left(\frac{2c_s^2}{s^2}\right)} \frac{1}{(\Delta x_3)^2} (t_{m,n,l-1} - 2t_{m,n,l} + t_{m,n,l+1}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_1} (r_{0,1;m-1,n,l} - r_{0,1;m+1,n,l})
\end{aligned}$$

$$\begin{aligned}
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_2} (r_{0,2;m,n-1,l} - r_{0,2;m,n+1,l}) \\
& - \overline{\left(\frac{\lambda s c_s}{2\mu c_p^2}\right)} \frac{1}{2\Delta x_3} (r_{0,3;m,n,l-1} - r_{0,3;m,n,l+1}) \\
& - \overline{\left(\frac{c_s}{s}\right)} \frac{1}{(\Delta x_3)^2} (d_{m,n,l-1} - 2d_{m,n,l} + d_{m,n,l+1}), \tag{B.13}
\end{aligned}$$

$$\begin{aligned}
F_{1,2;m,n,l}^{\text{p},M} &= \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_1 \Delta x_2} (r_{1,1;m-1,n-1,l} - r_{1,1;m-1,n+1,l} - r_{1,1;m+1,n-1,l} + r_{1,1;m+1,n+1,l}) \\
&+ \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_1 \Delta x_2} (r_{2,2;m-1,n-1,l} - r_{2,2;m-1,n+1,l} - r_{2,2;m+1,n-1,l} + r_{2,2;m+1,n+1,l}) \\
&+ \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_1 \Delta x_2} (r_{3,3;m-1,n-1,l} - r_{3,3;m-1,n+1,l} - r_{3,3;m+1,n-1,l} + r_{3,3;m+1,n+1,l}) \\
&+ \overline{\left(\frac{2c_s^2}{s^2}\right)} \frac{1}{2\Delta x_1 \Delta x_2} (t_{m-1,n-1,l} - t_{m-1,n+1,l} - t_{m+1,n-1,l} + t_{m+1,n+1,l}) \\
&- \overline{\left(\frac{c_s}{s}\right)} \frac{1}{2\Delta x_1 \Delta x_2} (d_{m-1,n-1,l} - d_{m-1,n+1,l} - d_{m+1,n-1,l} + d_{m+1,n+1,l}), \tag{B.14}
\end{aligned}$$

$$\begin{aligned}
F_{1,3;m,n,l}^{\text{p},M} &= \frac{1}{2\Delta x_1 \Delta x_3} (r_{1,1;m-1,n,l-1} - r_{1,1;m-1,n,l+1} - r_{1,1;m+1,n,l-1} + r_{1,1;m+1,n,l+1}) \\
&+ \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_1 \Delta x_3} (r_{2,2;m-1,n,l-1} - r_{2,2;m-1,n,l+1} - r_{2,2;m+1,n,l-1} + r_{2,2;m+1,n,l+1}) \\
&+ \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_1 \Delta x_3} (r_{3,3;m-1,n,l-1} - r_{3,3;m-1,n,l+1} - r_{3,3;m+1,n,l-1} + r_{3,3;m+1,n,l+1}) \\
&+ \overline{\left(\frac{2c_s^2}{s^2}\right)} \frac{1}{2\Delta x_1 \Delta x_3} (t_{m-1,n,l-1} - t_{m-1,n,l+1} - t_{m+1,n,l-1} + t_{m+1,n,l+1}) \\
&- \overline{\left(\frac{c_s}{s}\right)} \frac{1}{2\Delta x_1 \Delta x_3} (d_{m-1,n,l-1} - d_{m-1,n,l+1} - d_{m+1,n,l-1} + d_{m+1,n,l+1}), \tag{B.15}
\end{aligned}$$

$$\begin{aligned}
F_{2,3;m,n,l}^{\text{p},M} &= \frac{1}{2\Delta x_2 \Delta x_3} (r_{1,1;m,n-1,l-1} - r_{1,1;m,n-1,l+1} - r_{1,1;m,n+1,l-1} + r_{1,1;m,n+1,l+1}) \\
&+ \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_2 \Delta x_3} (r_{2,2;m,n-1,l-1} - r_{2,2;m,n-1,l+1} - r_{2,2;m,n+1,l-1} + r_{2,2;m,n+1,l+1}) \\
&+ \overline{\left(\frac{\lambda}{\rho c_p^2}\right)} \frac{1}{2\Delta x_2 \Delta x_3} (r_{3,3;m,n-1,l-1} - r_{3,3;m,n-1,l+1} - r_{3,3;m,n+1,l-1} + r_{3,3;m,n+1,l+1})
\end{aligned}$$

$$\begin{aligned}
& + \left( \frac{2c_s^2}{s^2} \right) \frac{1}{2\Delta x_2 \Delta x_3} (t_{m,n-1,l-1} - t_{m,n-1,l+1} - t_{m,n+1,l-1} + t_{m,n+1,l+1}) \\
& - \left( \frac{c_s}{s} \right) \frac{1}{2\Delta x_2 \Delta x_3} (d_{m,n-1,l-1} - d_{m,n-1,l+1} - d_{m,n+1,l-1} + d_{m,n+1,l+1}), \quad (\text{B.16})
\end{aligned}$$

$$\begin{aligned}
F_{1,1;m,n,l}^{\text{s},M} &= \frac{2}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\
& - \left( \frac{2c_s^2}{s^2} \right) \frac{1}{(\Delta x_1)^2} (t_{m-1,n,l} - 2t_{m,n,l} + t_{m+1,n,l}) \\
& - \left( \frac{s\rho c_s}{\mu} \right) \frac{1}{2\Delta x_1} (r_{0,1;m-1,n,l} - r_{0,1;m+1,n,l}) \\
& + \left( \frac{c_s}{s} \right) \frac{1}{(\Delta x_1)^2} (d_{m-1,n,l} - 2d_{m,n,l} + d_{m+1,n,l}), \quad (\text{B.17})
\end{aligned}$$

$$\begin{aligned}
F_{2,2;m,n,l}^{\text{s},M} &= \frac{2}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\
& + \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n-1,l+1} - r_{2,3;m,n+1,l-1} + r_{2,3;m,n+1,l+1}) \\
& - \left( \frac{2c_s^2}{s^2} \right) \frac{1}{(\Delta x_2)^2} (t_{m,n-1,l} - 2t_{m,n,l} + t_{m,n+1,l}) \\
& - \left( \frac{s\rho c_s}{\mu} \right) \frac{1}{2\Delta x_2} (r_{0,2;m,n-1,l} - r_{0,2;m,n+1,l}) \\
& + \left( \frac{c_s}{s} \right) \frac{1}{(\Delta x_2)^2} (d_{m,n-1,l} - 2d_{m,n,l} + d_{m,n+1,l}), \quad (\text{B.18})
\end{aligned}$$

$$\begin{aligned}
F_{3,3;m,n,l}^{\text{s},M} &= \frac{2}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{3,3;m,n,l} + r_{3,3;m,n,l+1}) \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\
& + \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n-1,l+1} - r_{2,3;m,n+1,l-1} + r_{2,3;m,n+1,l+1})
\end{aligned}$$

$$\begin{aligned}
& -\left(\frac{2c_s^2}{s^2}\right) \frac{1}{(\Delta x_3)^2} (t_{m,n,l-1} - 2t_{m,n,l} + t_{m,n,l+1}) \\
& -\left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_3} (r_{0,3;m,n,l-1} - r_{0,3;m,n,l+1}) \\
& +\left(\frac{c_s}{s}\right) \frac{1}{(\Delta x_3)^2} (d_{m,n,l-1} - 2d_{m,n,l} + d_{m,n,l+1}), \tag{B.19}
\end{aligned}$$

$$\begin{aligned}
F_{1,2;m,n,l}^{\text{s},M} = & \frac{1}{2\Delta x_1 \Delta x_2} (r_{1,1;m-1,n-1,l} - r_{1,1;m-1,n+1,l} - r_{1,1;m+1,n-1,l} + r_{1,1;m+1,n+1,l}) \\
& + \frac{1}{2\Delta x_1 \Delta x_2} (r_{2,2;m-1,n-1,l} - r_{2,2;m-1,n+1,l} - r_{2,2;m+1,n-1,l} + r_{2,2;m+1,n+1,l}) \\
& + \frac{1}{(\Delta x_1)^2} (r_{1,2;m-1,n,l} - 2r_{1,2;m,n,l} + r_{1,2;m+1,n,l}) \\
& + \frac{1}{(\Delta x_2)^2} (r_{1,2;m,n-1,l} - 2r_{1,2;m,n,l} + r_{1,2;m,n+1,l}) \\
& + \frac{1}{4\Delta x_2 \Delta x_3} (r_{1,3;m,n-1,l-1} - r_{1,3;m,n-1,l+1} - r_{1,3;m,n+1,l-1} + r_{1,3;m,n+1,l+1}) \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{2,3;m-1,n,l-1} - r_{2,3;m-1,n,l+1} - r_{2,3;m+1,n,l-1} + r_{2,3;m+1,n,l+1}) \\
& -\left(\frac{2c_s^2}{s^2}\right) \frac{1}{2\Delta x_1 \Delta x_2} (t_{m-1,n-1,l} - t_{m-1,n+1,l} - t_{m+1,n-1,l} + t_{m+1,n+1,l}) \\
& -\left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_2} (r_{0,1;m,n-1,l} - r_{0,1;m,n+1,l}) \\
& -\left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_1} (r_{0,2;m-1,n,l} - r_{0,2;m+1,n,l}) \\
& +\left(\frac{c_s}{s}\right) \frac{1}{2\Delta x_1 \Delta x_2} (d_{m-1,n-1,l} - d_{m-1,n+1,l} - d_{m+1,n-1,l} + d_{m+1,n+1,l}), \tag{B.20}
\end{aligned}$$

$$\begin{aligned}
F_{1,3;m,n,l}^{\text{s},M} = & \frac{1}{2\Delta x_1 \Delta x_3} (r_{1,1;m-1,n,l-1} - r_{1,1;m-1,n,l+1} - r_{1,1;m+1,n,l-1} + r_{1,1;m+1,n,l+1}) \\
& + \frac{1}{2\Delta x_1 \Delta x_3} (r_{3,3;m-1,n,l-1} - r_{3,3;m-1,n,l+1} - r_{3,3;m+1,n,l-1} + r_{3,3;m+1,n,l+1}) \\
& + \frac{1}{4\Delta x_2 \Delta x_3} (r_{1,2;m,n-1,l-1} - r_{1,2;m,n-1,l+1} - r_{1,2;m,n+1,l-1} + r_{1,2;m,n+1,l+1}) \\
& + \frac{1}{(\Delta x_1)^2} (r_{1,3;m-1,n,l} - 2r_{1,3;m,n,l} + r_{1,3;m+1,n,l}) \\
& + \frac{1}{(\Delta x_3)^2} (r_{1,3;m,n,l-1} - 2r_{1,3;m,n,l} + r_{1,3;m,n,l+1})
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{2,3;m-1,n-1,l} - r_{2,3;m-1,n+1,l} - r_{2,3;m+1,n-1,l} + r_{2,3;m+1,n+1,l}) \\
& - \left(\frac{2c_s^2}{s^2}\right) \frac{1}{2\Delta x_1 \Delta x_3} (t_{m-1,n,l-1} - t_{m-1,n,l+1} - t_{m+1,n,l-1} + t_{m+1,n,l+1}) \\
& - \left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_3} (r_{0,1;m,n,l-1} - r_{0,1;m,n,l+1}) \\
& - \left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_1} (r_{0,3;m-1,n,l} - r_{0,3;m+1,n,l}) \\
& + \left(\frac{c_s}{s}\right) \frac{1}{2\Delta x_1 \Delta x_3} (d_{m-1,n,l-1} - d_{m-1,n,l+1} - d_{m+1,n,l-1} + d_{m+1,n,l+1}) \quad (\mathbf{B}, 21)
\end{aligned}$$

$$\begin{aligned}
F_{2,3;m,n,l}^{S,M} & = \frac{1}{2\Delta x_2 \Delta x_3} (r_{2,2;m,n-1,l-1} - r_{2,2;m,n-1,l+1} - r_{2,2;m,n+1,l-1} + r_{2,2;m,n+1,l+1}) \\
& + \frac{1}{2\Delta x_2 \Delta x_3} (r_{3,3;m,n-1,l-1} - r_{3,3;m,n-1,l+1} - r_{3,3;m,n+1,l-1} + r_{3,3;m,n+1,l+1}) \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,2;m-1,n,l-1} - r_{1,2;m-1,n,l+1} - r_{1,2;m+1,n,l-1} + r_{1,2;m+1,n,l+1}) \\
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,3;m-1,n-1,l} - r_{1,3;m-1,n+1,l} - r_{1,3;m+1,n-1,l} + r_{1,3;m+1,n+1,l}) \\
& + \frac{1}{(\Delta x_2)^2} (r_{2,3;m,n-1,l} - 2r_{2,3;m,n,l} + r_{2,3;m,n+1,l}) \\
& + \frac{1}{(\Delta x_3)^2} (r_{2,3;m,n,l-1} - 2r_{2,3;m,n,l} + r_{2,3;m,n,l+1}) \\
& - \left(\frac{2c_s^2}{s^2}\right) \frac{1}{2\Delta x_2 \Delta x_3} (t_{m,n-1,l-1} - t_{m,n-1,l+1} - t_{m,n+1,l-1} + t_{m,n+1,l+1}) \\
& - \left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_3} (r_{0,2;m,n,l-1} - r_{0,2;m,n,l+1}) \\
& - \left(\frac{s\rho c_s}{\mu}\right) \frac{1}{2\Delta x_2} (r_{0,3;m,n-1,l} - r_{0,3;m,n+1,l}) \\
& + \left(\frac{c_s}{s}\right) \frac{1}{2\Delta x_2 \Delta x_3} (d_{m,n-1,l-1} - d_{m,n-1,l+1} - d_{m,n+1,l-1} + d_{m,n+1,l+1}) \quad (\mathbf{B}, 22)
\end{aligned}$$

$$\begin{aligned}
F_{0,1;m,n,l}^{P,\rho} & = \left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right) \frac{1}{2\Delta x_1} (r_{1,1;m-1,n,l} - r_{1,1;m+1,n,l}) \\
& + \left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right) \frac{1}{2\Delta x_1} (r_{2,2;m-1,n,l} - r_{2,2;m+1,n,l}) \\
& + \left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right) \frac{1}{2\Delta x_1} (r_{3,3;m-1,n,l} - r_{3,3;m+1,n,l})
\end{aligned}$$

$$\begin{aligned}
& + \overline{\left(\frac{2\mu}{s\rho c_s}\right)} \frac{1}{2\Delta x_1} (t_{m-1,n,l} - t_{m+1,n,l}) \\
& - \frac{1}{(\Delta x_1)^2} (r_{0,1;m-1,n,l} - 2r_{0,1;m,n,l} + r_{0,1;m+1,n,l}) \\
& - \frac{1}{4\Delta x_1 \Delta x_2} (r_{0,2;m-1,n-1,l} - r_{0,2;m-1,n+1,l} - r_{0,2;m+1,n-1,l} + r_{0,2;m+1,n+1,l}) \\
& - \frac{1}{4\Delta x_1 \Delta x_3} (r_{0,3;m-1,n,l-1} - r_{0,3;m-1,n,l+1} - r_{0,3;m+1,n,l-1} + r_{0,3;m+1,n,l+1}),
\end{aligned} \tag{B.23}$$

$$\begin{aligned}
F_{0,2;m,n,l}^{\text{P},\rho} & = \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right)} \frac{1}{2\Delta x_2} (r_{1,1;m,n-1,l} - r_{1,1;m,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right)} \frac{1}{2\Delta x_2} (r_{2,2;m,n-1,l} - r_{2,2;m,n+1,l}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right)} \frac{1}{2\Delta x_2} (r_{3,3;m,n-1,l} - r_{3,3;m,n+1,l}) \\
& + \overline{\left(\frac{2\mu}{s\rho c_s}\right)} \frac{1}{2\Delta x_2} (t_{m,n-1,l} - t_{m,n+1,l}) \\
& - \frac{1}{4\Delta x_1 \Delta x_2} (r_{0,1;m-1,n-1,l} - r_{0,1;m-1,n+1,l} - r_{0,1;m+1,n-1,l} + r_{0,1;m+1,n+1,l}) \\
& - \frac{1}{(\Delta x_2)^2} (r_{0,2;m,n-1,l} - 2r_{0,2;m,n,l} + r_{0,2;m,n+1,l}) \\
& - \frac{1}{4\Delta x_2 \Delta x_3} (r_{0,3;m,n-1,l-1} - r_{0,3;m,n-1,l+1} - r_{0,3;m,n+1,l-1} + r_{0,3;m,n+1,l+1}),
\end{aligned} \tag{B.24}$$

$$\begin{aligned}
F_{0,3;m,n,l}^{\text{P},\rho} & = \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right)} \frac{1}{2\Delta x_3} (r_{1,1;m,n,l-1} - r_{1,1;m,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right)} \frac{1}{2\Delta x_3} (r_{2,2;m,n,l-1} - r_{2,2;m,n,l+1}) \\
& + \overline{\left(\frac{\lambda}{\rho c_p^2} \frac{s}{c_s}\right)} \frac{1}{2\Delta x_3} (r_{3,3;m,n,l-1} - r_{3,3;m,n,l+1}) \\
& + \overline{\left(\frac{2\mu}{s\rho c_s}\right)} \frac{1}{2\Delta x_3} (t_{m,n,l-1} - t_{m,n,l+1}) \\
& - \frac{1}{4\Delta x_1 \Delta x_3} (r_{0,1;m-1,n,l-1} - r_{0,1;m-1,n,l+1} - r_{0,1;m+1,n,l-1} + r_{0,1;m+1,n,l+1})
\end{aligned}$$

$$\begin{aligned}
& - \frac{1}{4\Delta x_2 \Delta x_3} (r_{0,2;m,n-1,l-1} - r_{0,2;m,n-1,l+1} - r_{0,2;m,n+1,l-1} + r_{0,2;m,n+1,l+1}) \\
& - \frac{1}{(\Delta x_3)^2} (r_{0,3;m,n,l-1} - 2r_{0,3;m,n,l} + r_{0,3;m,n,l+1}),
\end{aligned} \tag{B.25}$$

$$\begin{aligned}
F_{0,1;m,n,l}^{s,\rho} = & \overline{\left(\frac{2s}{c_s}\right)} \frac{1}{2\Delta x_1} (r_{1,1;m-1,n,l} - r_{1,1;m+1,n,l}) \\
& + \overline{\left(\frac{s}{c_s}\right)} \frac{1}{2\Delta x_2} (r_{1,2;m,n-1,l} - r_{1,2;m,n+1,l}) \\
& + \overline{\left(\frac{s}{c_s}\right)} \frac{1}{2\Delta x_3} (r_{1,3;m,n,l-1} - r_{1,3;m,n,l+1}) \\
& - \overline{\left(\frac{2\mu}{s\rho c_s}\right)} \frac{1}{2\Delta x_1} (t_{m-1,n,l} - t_{m+1,n,l}) \\
& - \overline{\left(\frac{s^2}{c_s^2}\right)} r_{0,1;m,n,l} \\
& + \frac{1}{(\Delta x_1)^2} (r_{0,1;m-1,n,l} - 2r_{0,1;m,n,l} + r_{0,1;m+1,n,l}) \\
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{0,2;m-1,n-1,l} - r_{0,2;m-1,n+1,l} - r_{0,2;m+1,n-1,l} + r_{0,2;m+1,n+1,l}) \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{0,3;m-1,n,l-1} - r_{0,3;m-1,n,l+1} - r_{0,3;m+1,n,l-1} + r_{0,3;m+1,n,l+1}),
\end{aligned} \tag{B.26}$$

$$\begin{aligned}
F_{0,2;m,n,l}^{s,\rho} = & \overline{\left(\frac{2s}{c_s}\right)} \frac{1}{2\Delta x_2} (r_{2,2;m,n-1,l} - r_{2,2;m,n+1,l}) \\
& + \overline{\left(\frac{s}{c_s}\right)} \frac{1}{2\Delta x_1} (r_{1,2;m-1,n,l} - r_{1,2;m+1,n,l}) \\
& + \overline{\left(\frac{s}{c_s}\right)} \frac{1}{2\Delta x_3} (r_{2,3;m,n,l-1} - r_{2,3;m,n,l+1}) \\
& - \overline{\left(\frac{2\mu}{s\rho c_s}\right)} \frac{1}{2\Delta x_2} (t_{m,n-1,l} - t_{m,n+1,l}) \\
& - \overline{\left(\frac{s^2}{c_s^2}\right)} r_{0,2;m,n,l} \\
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{0,1;m-1,n-1,l} - r_{0,1;m-1,n+1,l} - r_{0,1;m+1,n-1,l} + r_{0,1;m+1,n+1,l}) \\
& + \frac{1}{(\Delta x_2)^2} (r_{0,2;m,n-1,l} - 2r_{0,2;m,n,l} + r_{0,2;m,n+1,l})
\end{aligned}$$

$$+ \frac{1}{4\Delta x_2 \Delta x_3} (r_{0,3;m,n-1,l-1} - r_{0,3;m,n-1,l+1} - r_{0,3;m,n+1,l-1} + r_{0,3;m,n+1,l+1}), \quad (\text{B.27})$$

$$\begin{aligned}
F_{0,3;m,n,l}^{s,\rho} = & \overline{\left(\frac{2s}{c_s}\right)} \frac{1}{2\Delta x_3} (r_{3,3;m,n,l-1} - r_{3,3;m,n,l+1}) \\
& + \overline{\left(\frac{s}{c_s}\right)} \frac{1}{2\Delta x_1} (r_{1,3;m-1,n,l} - r_{1,3;m+1,n,l}) \\
& + \overline{\left(\frac{s}{c_s}\right)} \frac{1}{2\Delta x_2} (r_{2,3;m,n-1,l} - r_{2,3;m,n+1,l}) \\
& - \overline{\left(\frac{2\mu}{s\rho c_s}\right)} \frac{1}{2\Delta x_3} (t_{m,n,l-1} - t_{m,n,l+1}) \\
& - \overline{\left(\frac{s^2}{c_s^2}\right)} r_{0,3;m,n,l} \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{0,1;m-1,n,l-1} - r_{0,1;m-1,n,l+1} - r_{0,1;m+1,n,l-1} + r_{0,1;m+1,n,l+1}) \\
& + \frac{1}{4\Delta x_2 \Delta x_3} (r_{0,2;m,n-1,l-1} - r_{0,2;m,n-1,l+1} - r_{0,2;m,n+1,l-1} + r_{0,2;m,n+1,l+1}) \\
& + \frac{1}{(\Delta x_3)^2} (r_{0,3;m,n,l-1} - 2r_{0,3;m,n,l} + r_{0,3;m,n,l+1}), \quad (\text{B.28})
\end{aligned}$$

where

$$\begin{aligned}
t_{m,n,l} = & \frac{1}{(\Delta x_1)^2} (r_{1,1;m-1,n,l} - 2r_{1,1;m,n,l} + r_{1,1;m+1,n,l}) \\
& + \frac{1}{(\Delta x_2)^2} (r_{2,2;m,n-1,l} - 2r_{2,2;m,n,l} + r_{2,2;m,n+1,l}) \\
& + \frac{1}{(\Delta x_3)^2} (r_{3,3;m,n,l-1} - 2r_{3,3;m,n,l} + r_{3,3;m,n,l+1}) \\
& + \frac{1}{4\Delta x_1 \Delta x_2} (r_{1,2;m-1,n-1,l} - r_{1,2;m-1,n+1,l} - r_{1,2;m+1,n-1,l} + r_{1,2;m+1,n+1,l}) \\
& + \frac{1}{4\Delta x_1 \Delta x_3} (r_{1,3;m-1,n,l-1} - r_{1,3;m-1,n,l+1} - r_{1,3;m+1,n,l-1} + r_{1,3;m+1,n,l+1}) \\
& + \frac{1}{4\Delta x_2 \Delta x_3} (r_{2,3;m,n-1,l-1} - r_{2,3;m,n-1,l+1} - r_{2,3;m,n+1,l-1} + r_{2,3;m,n+1,l+1}), \quad (\text{B.29})
\end{aligned}$$

$$\begin{aligned}
d_{m,n,l} &= \frac{1}{2\Delta x_1} (r_{0,1;m-1,n,l} - r_{0,1;m+1,n,l}) \\
&\quad + \frac{1}{2\Delta x_2} (r_{0,2;m,n-1,l} - r_{0,2;m,n+1,l}) \\
&\quad + \frac{1}{2\Delta x_3} (r_{0,3;m,n,l-1} - r_{0,3;m,n,l+1}), \tag{B.30}
\end{aligned}$$

for  $m = -2, \dots, M+3$ ,  $n = -2, \dots, N+3$ , and  $l = -2, \dots, L+3$ , and

$$\begin{aligned}
r_{p,q;m,n,l} &= 0, \quad m = -3, -2, -1, 0, M+1, M+2, M+3, M+4, \quad \forall n, \forall l, \\
r_{p,q;m,n,l} &= 0, \quad n = -3, -2, -1, 0, N+1, N+2, N+3, N+4, \quad \forall m, \forall l, \\
r_{p,q;m,n,l} &= 0, \quad l = -3, -2, -1, 0, L+1, L+2, L+3, L+4, \quad \forall m, \forall n. \tag{B.31}
\end{aligned}$$

## C Complete explicit expression of diagonal pre-conditioner

The diagonal matrix  $\mathcal{D}$  is recognized as

$$\begin{aligned}
\mathcal{D}_{1,1;m,n,l} &= 1 + \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^\Lambda + \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^\Lambda \\
&\quad + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\Lambda (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
&\quad - \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^M \\
&\quad - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
&\quad - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\
&\quad - 2 \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s) \\
&\quad - \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_1)^2} \left[ \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^p - 2\mathcal{G}_{-1,0,0}^p + \mathcal{G}_{0,0,0}^p) \right. \\
&\quad \left. - 2 \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \right. \\
&\quad \left. + \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - 2\mathcal{G}_{1,0,0}^p + \mathcal{G}_{2,0,0}^p) \right] \\
&\quad + \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_1)^2} \left[ \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^s - 2\mathcal{G}_{-1,0,0}^s + \mathcal{G}_{0,0,0}^s) \right.
\end{aligned}$$

$$\begin{aligned}
& -2 \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s) \\
& + \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - 2\mathcal{G}_{1,0,0}^s + \mathcal{G}_{2,0,0}^s) \Big], \tag{C.1}
\end{aligned}$$

$$\begin{aligned}
\mathcal{D}_{2,2;m,n,l} = & 1 + \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^\Lambda + \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^\Lambda \\
& + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\Lambda (\mathcal{G}_{0,-1,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,1,0}^p) \\
& - \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^M \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,1,0}^p) \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,1,0}^p) \\
& - 2 \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,1,0}^s) \\
& - \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_2)^2} \left[ \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,0}^p - 2\mathcal{G}_{0,-1,0}^p + \mathcal{G}_{0,0,0}^p) \right. \\
& - 2 \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,1,0}^p) \\
& \left. + \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - 2\mathcal{G}_{0,1,0}^p + \mathcal{G}_{0,2,0}^p) \right] \\
& + \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_2)^2} \left[ \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,0}^s - 2\mathcal{G}_{0,-1,0}^s + \mathcal{G}_{0,0,0}^s) \right. \\
& - 2 \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,1,0}^s) \\
& \left. + \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - 2\mathcal{G}_{0,1,0}^s + \mathcal{G}_{0,2,0}^s) \right], \tag{C.2}
\end{aligned}$$

$$\begin{aligned}
\mathcal{D}_{3,3;m,n,l} = & 1 + \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^\Lambda + \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^\Lambda \\
& + \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\Lambda (\mathcal{G}_{0,0,-1}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,1}^p) \\
& - \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \chi_{m,n,l}^M - \frac{\lambda}{\rho c_p^2} \frac{\lambda s^2}{2\mu c_p^2} \Delta x_1 \Delta x_2 \Delta x_3 \mathcal{G}_{0,0,0}^p \chi_{m,n,l}^M
\end{aligned}$$

$$\begin{aligned}
& - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,1}^p) \\
& - \frac{\lambda}{\rho c_p^2} \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,1}^p) \\
& - 2 \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,1}^s) \\
& - \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_3)^2} \left[ \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-2}^p - 2\mathcal{G}_{0,0,-1}^p + \mathcal{G}_{0,0,0}^p) \right. \\
& - 2 \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,1}^p) \\
& \left. + \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - 2\mathcal{G}_{0,0,1}^p + \mathcal{G}_{0,0,2}^p) \right] \\
& + \frac{2c_s^2}{s^2} \frac{1}{(\Delta x_3)^2} \left[ \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-2}^s - 2\mathcal{G}_{0,0,-1}^s + \mathcal{G}_{0,0,0}^s) \right. \\
& - 2 \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,1}^s) \\
& \left. + \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - 2\mathcal{G}_{0,0,1}^s + \mathcal{G}_{0,0,2}^s) \right], \tag{C.3}
\end{aligned}$$

$$\begin{aligned}
\mathcal{D}_{1,2;m,n,l} &= 1 - \chi_{m,n,l}^M \\
& - \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s) \\
& - \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,1,0}^s) \\
& - \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_1 \Delta x_2} \left[ \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,-2,0}^p - \mathcal{G}_{-2,0,0}^p - \mathcal{G}_{0,-2,0}^p + \mathcal{G}_{0,0,0}^p) \right. \\
& - \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^p - \mathcal{G}_{-2,2,0}^p - \mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,2,0}^p) \\
& - \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,0}^p - \mathcal{G}_{0,0,0}^p - \mathcal{G}_{2,-2,0}^p + \mathcal{G}_{2,0,0}^p) \\
& \left. + \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - \mathcal{G}_{2,0,0}^p - \mathcal{G}_{0,2,0}^p + \mathcal{G}_{2,2,0}^p) \right] \\
& + \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_1 \Delta x_2} \left[ \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,-2,0}^s - \mathcal{G}_{-2,0,0}^s - \mathcal{G}_{0,-2,0}^s + \mathcal{G}_{0,0,0}^s) \right. \\
& - \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^s - \mathcal{G}_{-2,2,0}^s - \mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,2,0}^s) \\
& - \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,0}^s - \mathcal{G}_{0,0,0}^s - \mathcal{G}_{2,-2,0}^s + \mathcal{G}_{2,0,0}^s) \\
& \left. + \frac{1}{2\Delta x_1 \Delta x_2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - \mathcal{G}_{2,0,0}^s - \mathcal{G}_{0,2,0}^s + \mathcal{G}_{2,2,0}^s) \right], \tag{C.4}
\end{aligned}$$

$$\begin{aligned}
\mathcal{D}_{1,3;m,n,l} &= 1 - \chi_{m,n,l}^M \\
&- \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s) \\
&- \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,1}^s) \\
&- \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_1 \Delta x_3} \left[ \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,-2}^p - \mathcal{G}_{-2,0,0}^p - \mathcal{G}_{0,0,-2}^p + \mathcal{G}_{0,0,0}^p) \right. \\
&- \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^p - \mathcal{G}_{-2,0,2}^p - \mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,2}^p) \\
&- \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-2}^p - \mathcal{G}_{0,0,0}^p - \mathcal{G}_{2,0,-2}^p + \mathcal{G}_{2,0,0}^p) \\
&\left. + \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - \mathcal{G}_{2,0,0}^p - \mathcal{G}_{0,0,2}^p + \mathcal{G}_{2,0,2}^p) \right] \\
&+ \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_1 \Delta x_3} \left[ \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,-2}^s - \mathcal{G}_{-2,0,0}^s - \mathcal{G}_{0,0,-2}^s + \mathcal{G}_{0,0,0}^s) \right. \\
&- \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{-2,0,0}^s - \mathcal{G}_{-2,0,2}^s - \mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,2}^s) \\
&- \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-2}^s - \mathcal{G}_{0,0,0}^s - \mathcal{G}_{2,0,-2}^s + \mathcal{G}_{2,0,0}^s) \\
&\left. + \frac{1}{2\Delta x_1 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - \mathcal{G}_{2,0,0}^s - \mathcal{G}_{0,0,2}^s + \mathcal{G}_{2,0,2}^s) \right], \tag{C.5}
\end{aligned}$$

$$\begin{aligned}
\mathcal{D}_{2,3;m,n,l} &= 1 - \chi_{m,n,l}^M \\
&- \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-1,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,1,0}^s) \\
&- \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-1}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,1}^s) \\
&- \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_2 \Delta x_3} \left[ \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,-2}^p - \mathcal{G}_{0,-2,0}^p - \mathcal{G}_{0,0,-2}^p + \mathcal{G}_{0,0,0}^p) \right. \\
&- \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,0}^p - \mathcal{G}_{0,-2,2}^p - \mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,2}^p) \\
&- \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-2}^p - \mathcal{G}_{0,0,0}^p - \mathcal{G}_{0,2,-2}^p + \mathcal{G}_{0,2,0}^p) \\
&\left. + \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^p - \mathcal{G}_{0,2,0}^p - \mathcal{G}_{0,0,2}^p + \mathcal{G}_{0,2,2}^p) \right] \\
&+ \frac{2c_s^2}{s^2} \frac{1}{4\Delta x_2 \Delta x_3} \left[ \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,-2}^s - \mathcal{G}_{0,-2,0}^s - \mathcal{G}_{0,0,-2}^s + \mathcal{G}_{0,0,0}^s) \right. \\
&- \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,-2,0}^s - \mathcal{G}_{0,-2,2}^s - \mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,2}^s) \\
&- \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,-2}^s - \mathcal{G}_{0,0,0}^s - \mathcal{G}_{0,2,-2}^s + \mathcal{G}_{0,2,0}^s) \\
&\left. + \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - \mathcal{G}_{0,2,0}^s - \mathcal{G}_{0,0,2}^s + \mathcal{G}_{0,2,2}^s) \right]
\end{aligned}$$

$$+ \frac{1}{2\Delta x_2 \Delta x_3} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^M (\mathcal{G}_{0,0,0}^s - \mathcal{G}_{0,2,0}^s - \mathcal{G}_{0,0,2}^s + \mathcal{G}_{0,2,2}^s) \Big], \quad (\text{C.6})$$

$$\begin{aligned} \mathcal{D}_{0,1;m,n,l} &= 1 + \frac{s^2}{c_s^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho \mathcal{G}_{0,0,0}^s \\ &+ \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho (\mathcal{G}_{-1,0,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{1,0,0}^p) \\ &- \frac{1}{(\Delta x_1)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho (\mathcal{G}_{-1,0,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{1,0,0}^s), \end{aligned} \quad (\text{C.7})$$

$$\begin{aligned} \mathcal{D}_{0,2;m,n,l} &= 1 + \frac{s^2}{c_s^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho \mathcal{G}_{0,0,0}^s \\ &+ \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho (\mathcal{G}_{0,-1,0}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,1,0}^p) \\ &- \frac{1}{(\Delta x_2)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho (\mathcal{G}_{0,-1,0}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,1,0}^s), \end{aligned} \quad (\text{C.8})$$

and

$$\begin{aligned} \mathcal{D}_{0,3;m,n,l} &= 1 + \frac{s^2}{c_s^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho \mathcal{G}_{0,0,0}^s \\ &+ \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho (\mathcal{G}_{0,0,-1}^p - 2\mathcal{G}_{0,0,0}^p + \mathcal{G}_{0,0,1}^p) \\ &- \frac{1}{(\Delta x_3)^2} \Delta x_1 \Delta x_2 \Delta x_3 \chi_{m,n,l}^\rho (\mathcal{G}_{0,0,-1}^s - 2\mathcal{G}_{0,0,0}^s + \mathcal{G}_{0,0,1}^s), \end{aligned} \quad (\text{C.9})$$

Therefore, the explicit express of the diagonal pre-conditioner is given by

$$(\mathcal{D}^{-1})_{p,q;m,n,l} = (\mathcal{D}_{p,q;m,n,l})^{-1}. \quad (\text{C.10})$$

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