## Supplement of

## Green's theorem in seismic imaging across the scales

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## S1 Classical homogeneous Green's function representation

## S1.1 Definition of the homogeneous Green's function

Consider an inhomogeneous lossless acoustic medium with mass density $\rho(\boldsymbol{x})$ and compressibility $\kappa(\boldsymbol{x})$. In this medium a space- and time-dependent source distribution $q(\boldsymbol{x}, t)$ is present, with $q$ defined as the volume-injection rate density. The acoustic wave field, caused by this source distribution, is described in terms of the acoustic pressure $p(\boldsymbol{x}, t)$ and the particle velocity $v_{i}(\boldsymbol{x}, t)$. These field quantities obey the equation of motion and the stress-strain relation, according to

$$
\begin{align*}
\rho \partial_{t} v_{i}+\partial_{i} p & =0  \tag{S1}\\
\kappa \partial_{t} p+\partial_{i} v_{i} & =q \tag{S2}
\end{align*}
$$

When $q$ is an impulsive source at $\boldsymbol{x}=\boldsymbol{x}_{\mathrm{A}}$ and $t=0$, according to

$$
\begin{equation*}
q(\boldsymbol{x}, t)=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{A}}\right) \delta(t) \tag{S3}
\end{equation*}
$$

then the causal solution of Eqs. (S1) and (S2) defines the Green's function, hence

$$
\begin{equation*}
p(\boldsymbol{x}, t)=G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, t\right) . \tag{S4}
\end{equation*}
$$

By eliminating $v_{i}$ from Eqs. (S1) and (S2) and substituting Eqs. (S3) and (S4), we find that the Green's function $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, t\right)$ obeys the following wave equation

$$
\begin{equation*}
\partial_{i}\left(\rho^{-1} \partial_{i} G\right)-\kappa \partial_{t}^{2} G=-\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{A}}\right) \partial_{t} \delta(t) \tag{S5}
\end{equation*}
$$

Wave equation (S5) is symmetric in time, except for the source on the right-hand side, which is anti-symmetric. Hence, the time-reversed Green's function $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}},-t\right)$ obeys the same wave equation, but with opposite sign for the source. By summing the wave equations for $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, t\right)$ and $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}},-t\right)$, the sources on the right-hand sides cancel each other, hence, the homogeneous Green's function

$$
\begin{equation*}
G_{\mathrm{h}}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, t\right)=G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, t\right)+G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}},-t\right) \tag{S6}
\end{equation*}
$$

obeys the homogeneous equation

$$
\begin{equation*}
\partial_{i}\left(\rho^{-1} \partial_{i} G_{\mathrm{h}}\right)-\kappa \partial_{t}^{2} G_{\mathrm{h}}=0 \tag{S7}
\end{equation*}
$$

## S1.2 Reciprocity theorems

We define the temporal Fourier transform of a time-dependent quantity $u(t)$ as

$$
\begin{equation*}
u(\omega)=\int_{-\infty}^{\infty} u(t) \exp (i \omega t) \mathrm{d} t \tag{S8}
\end{equation*}
$$

In the frequency domain, Eqs. (S1) and (S2) transform to

$$
\begin{align*}
& -i \omega \rho v_{i}+\partial_{i} p=0  \tag{S9}\\
& -i \omega \kappa p+\partial_{i} v_{i}=q \tag{S10}
\end{align*}
$$

We introduce two independent acoustic states, which will be distinguished by subscripts A and B. Rayleigh's reciprocity theorem is obtained by considering the quantity $\partial_{i}\left\{p_{\mathrm{A}} v_{i, B}-v_{i, A} p_{\mathrm{B}}\right\}$, applying the product rule for differentiation, substituting Eqs. (S9) and (S10) for both states, integrating the result over a spatial domain $\mathbb{V}$ enclosed by surface $\mathbb{S}$ with outward pointing
normal $n_{i}$, and applying the theorem of Gauss (de Hoop, 1988; Fokkema and van den Berg, 1993). Assuming that in $\mathbb{V}$ the medium parameters $\rho(\boldsymbol{x})$ and $\kappa(\boldsymbol{x})$ in the two states are identical, this yields Rayleigh's reciprocity theorem of the convolution type

$$
\begin{equation*}
\int_{\mathrm{V}}\left\{p_{\mathrm{A}} q_{\mathrm{B}}-q_{\mathrm{A}} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\oint_{\mathbb{S}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}\left(\partial_{i} p_{\mathrm{B}}\right)-\left(\partial_{i} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right\} n_{i} \mathrm{~d} \boldsymbol{x} . \tag{S11}
\end{equation*}
$$

We derive a second form of Rayleigh's reciprocity theorem for time-reversed wave fields. In the frequency domain, timereversal is replaced by complex conjugation. When $p$ is a solution of Eqs. (S9) and (S10) with source distribution $q$ (and real-valued medium parameters), then $p^{*}$ obeys the same equations with source distribution $-q^{*}$. Making these substitutions for state A in Eq. (S11) we obtain Rayleigh's reciprocity theorem of the correlation type (Bojarski, 1983)

$$
\begin{equation*}
\int_{\mathrm{V}}\left\{p_{\mathrm{A}}^{*} q_{\mathrm{B}}+q_{\mathrm{A}}^{*} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\oint_{\mathbb{S}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}^{*}\left(\partial_{i} p_{\mathrm{B}}\right)-\left(\partial_{i} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right\} n_{i} \mathrm{~d} \boldsymbol{x} . \tag{S12}
\end{equation*}
$$

## S1.3 Representation of the homogeneous Green's function

We choose point sources in both states, according to $q_{\mathrm{A}}(\boldsymbol{x}, \omega)=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{A}}\right)$ and $q_{\mathrm{B}}(\boldsymbol{x}, \omega)=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right)$, with $\boldsymbol{x}_{\mathrm{A}}$ and $\boldsymbol{x}_{\mathrm{B}}$ both in $\mathbb{V}$. The fields in states A and B are thus expressed in terms of Green's functions, according to

$$
\begin{align*}
p_{\mathrm{A}}(\boldsymbol{x}, \omega) & =G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right),  \tag{S13}\\
p_{\mathrm{B}}(\boldsymbol{x}, \omega) & =G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right), \tag{S14}
\end{align*}
$$

with $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)$ and $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$ being the Fourier transforms of $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, t\right)$ and $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, t\right)$, respectively. Making these substitutions in Eq. (S12) and using source-receiver reciprocity of the Green's functions gives (Porter, 1970; Oristaglio, 1989; Wapenaar, 2004; Van Manen et al., 2005)

$$
\begin{equation*}
G_{\mathrm{h}}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=\oint_{\mathbb{S}} \frac{1}{i \omega \rho(\boldsymbol{x})}\left(\left\{\partial_{i} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\right\} G^{*}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)-G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{i} G^{*}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right) n_{i} \mathrm{~d} \boldsymbol{x}, \tag{S15}
\end{equation*}
$$

where $G_{\mathrm{h}}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)$ is the homogeneous Green's function in the frequency domain. It is defined as

$$
\begin{equation*}
G_{\mathrm{h}}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+G^{*}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=2 \Re\left\{G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}, \tag{S16}
\end{equation*}
$$

where $\Re$ denotes the real part. Equation (S15) is an exact representation for the homogeneous Green's function $G_{\mathrm{h}}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)$.
When $\mathbb{S}$ is sufficiently smooth and the medium outside $\mathbb{S}$ is homogeneous (with mass density $\rho_{0}$, compressibility $\kappa_{0}$ and propagation velocity $c_{0}=\left(\kappa_{0} \rho_{0}\right)^{-1 / 2}$ ), the two terms under the integral in Eq. (S15) are nearly identical (but opposite in sign), hence

$$
\begin{equation*}
G_{\mathrm{h}}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=-2 \oint_{\mathbb{S}} \frac{1}{i \omega \rho_{0}} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{i} G^{*}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right) n_{i} \mathrm{~d} \boldsymbol{x} . \tag{S17}
\end{equation*}
$$

The main approximation is that evanescent waves are neglected at $\mathbb{S}$ (Zheng et al., 2011; Wapenaar et al., 2011).

## S2 Single-sided homogeneous Green's function representations

## S2.1 Modification of the configuration

We replace the arbitrary closed surface $\mathbb{S}$ by a combination of two surfaces $\mathbb{S}_{0}$ and $\mathbb{S}_{A}$, as indicated in Fig. S1. Here $\mathbb{S}_{0}$ may be curved, but $\mathbb{S}_{\mathrm{A}}$ is a horizontal surface, with $\boldsymbol{n}=(0,0,1)$. The depth level of $\mathbb{S}_{\mathrm{A}}$ is defined as $x_{3, \mathrm{~A}}$ (which is equal to


Figure S1. Modified configuration. The surface $\mathbb{S}$ consists of the combination of surfaces $\mathbb{S}_{0}$ and $\mathbb{S}_{A}$.
the $x_{3}$-coordinate of the point $\boldsymbol{x}_{\mathrm{A}}$ ). The domain between surfaces $\mathbb{S}_{0}$ and $\mathbb{S}_{\mathrm{A}}$ is called $\mathbb{V}_{\mathrm{A}}$. For this configuration, reciprocity theorems (S11) and (S12) are replaced by

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left\{p_{\mathrm{A}} q_{\mathrm{B}}-q_{\mathrm{A}} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{0}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}\left(\partial_{i} p_{\mathrm{B}}\right)-\left(\partial_{i} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right\} n_{i} \mathrm{~d} \boldsymbol{x}+\int_{\mathbb{S}_{\mathrm{A}}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x} \tag{S18}
\end{equation*}
$$

and

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left\{p_{\mathrm{A}}^{*} q_{\mathrm{B}}+q_{\mathrm{A}}^{*} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{0}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}^{*}\left(\partial_{i} p_{\mathrm{B}}\right)-\left(\partial_{i} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right\} n_{i} \mathrm{~d} \boldsymbol{x}+\int_{\mathbb{S}_{\mathrm{A}}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}^{*}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x} \tag{S19}
\end{equation*}
$$

respectively. In the following we use these reciprocity theorems as the basis for deriving several versions of single-sided homogeneous Green's function representations, each time by applying decomposition to one or more of the integrals in these theorems. The theory of the decomposition of these integrals is discussed in Appendix A.

## S2.2 Single-sided homogeneous Green's function representation: general formulation

Substituting Eqs. (A37) and (A38) for the surface integrals at $\mathbb{S}_{\mathrm{A}}$ into Eqs. (S18) and (S19), we obtain

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left(p_{\mathrm{A}} q_{\mathrm{B}}-q_{\mathrm{A}} p_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{0}} \frac{1}{i \omega \rho}\left(p_{\mathrm{A}}\left(\partial_{i} p_{\mathrm{B}}\right)-\left(\partial_{i} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right) n_{i} \mathrm{~d} \boldsymbol{x}-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right) p_{\mathrm{B}}^{-}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right) p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{S20}
\end{equation*}
$$

and, ignoring evanescent waves,

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left(p_{\mathrm{A}}^{*} q_{\mathrm{B}}+q_{\mathrm{A}}^{*} p_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{0}} \frac{1}{i \omega \rho}\left(p_{\mathrm{A}}^{*}\left(\partial_{i} p_{\mathrm{B}}\right)-\left(\partial_{i} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right) n_{i} \mathrm{~d} \boldsymbol{x}-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right)^{*} p_{\mathrm{B}}^{+}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right)^{*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} \tag{S21}
\end{equation*}
$$

For state A we consider the focusing function $f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)$, introduced in section 3.1 in "Green's theorem in seismic imaging across the scales". This focusing function is defined in a truncated version of the medium, which is identical to the actual medium in $\mathbb{V}_{A}$, but reflection free above $\mathbb{S}_{0}$ and below $\mathbb{S}_{A}$. Hence, the condition for the validity of Eqs. (A36), (A37) and (A38) is fulfilled at $\mathbb{S}_{\mathrm{A}}$. The focusing conditions at the focal plane $\mathbb{S}_{\mathrm{A}}$ are (Wapenaar et al., 2014)

$$
\begin{align*}
& {\left[\partial_{3} f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right]_{x_{3}=x_{3, \mathrm{~A}}}=\frac{1}{2} i \omega \rho\left(\boldsymbol{x}_{\mathrm{A}}\right) \delta\left(\boldsymbol{x}_{\mathrm{H}}-\boldsymbol{x}_{\mathrm{H}, \mathrm{~A}}\right),}  \tag{S22}\\
& {\left[\partial_{3} f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right]_{x_{3}=x_{3, \mathrm{~A}}}=0} \tag{S23}
\end{align*}
$$

For state B we consider the Green's function $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)=G^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+G^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$, with its source at $\boldsymbol{x}_{\mathrm{B}}$ anywhere in the half-space below $\mathbb{S}_{0}$. Note that the superscripts + and - in $f_{1}^{ \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)$ and $G^{ \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$ refer to the propagation direction (downward or upward) at the observation point $\boldsymbol{x}$. The source of the Green's function at $\boldsymbol{x}_{\mathrm{B}}$ is omnidirectional.

Substituting $q_{\mathrm{A}}(\boldsymbol{x}, \omega)=0, p_{\mathrm{A}}^{ \pm}(\boldsymbol{x}, \omega)=f_{1}^{ \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right), q_{\mathrm{B}}(\boldsymbol{x}, \omega)=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right)$ and $p_{\mathrm{B}}^{ \pm}(\boldsymbol{x}, \omega)=G^{ \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$ into Eqs. (S20) and (S21), using Eqs. (S22) and (S23), gives

$$
\begin{align*}
& G^{-}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+\chi\left(\boldsymbol{x}_{\mathrm{B}}\right) f_{1}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right) \\
& \quad=\int_{\mathbb{S}_{0}} \frac{1}{i \omega \rho(\boldsymbol{x})}\left(\left\{\partial_{i} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\right\} f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)-G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{i} f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right) n_{i} \mathrm{~d} \boldsymbol{x} \tag{S24}
\end{align*}
$$

and

$$
\begin{align*}
& G^{+}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)-\chi\left(\boldsymbol{x}_{\mathrm{B}}\right) f_{1}^{*}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right) \\
& \quad=-\int_{\mathrm{S}_{0}} \frac{1}{i \omega \rho(\boldsymbol{x})}\left(\left\{\partial_{i} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\right\} f_{1}^{*}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)-G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{i} f_{1}^{*}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right) n_{i} \mathrm{~d} \boldsymbol{x}, \tag{S25}
\end{align*}
$$

respectively, where $\chi$ is the characteristic function of the domain $\mathbb{V}_{\mathrm{A}}$. It is defined as

$$
\chi\left(\boldsymbol{x}_{\mathrm{B}}\right)= \begin{cases}1, & \text { for } \boldsymbol{x}_{\mathrm{B}} \text { between } \mathbb{S}_{0} \text { and } \mathbb{S}_{\mathrm{A}},  \tag{S26}\\ \frac{1}{2}, & \text { for } \boldsymbol{x}_{\mathrm{B}} \text { on } \mathbb{S}=\mathbb{S}_{0} \cup \mathbb{S}_{\mathrm{A}}, \\ 0, & \text { for } \boldsymbol{x}_{\mathrm{B}} \text { outside } \mathbb{S} .\end{cases}
$$

Summing Eqs. (S24) and (S25) and using source-receiver reciprocity for the Green's function on the left-hand side yields

$$
\begin{align*}
& G\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+\chi\left(\boldsymbol{x}_{\mathrm{B}}\right) 2 i \Im\left\{f_{1}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\} \\
& \quad=\int_{\mathrm{S}_{0}} \frac{2}{\omega \rho(\boldsymbol{x})}\left(\left\{\partial_{i} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\right\} \Im\left\{f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}-G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \Im\left\{\partial_{i} f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}\right) n_{i} \mathrm{~d} \boldsymbol{x}, \tag{S27}
\end{align*}
$$

where $\Im$ denotes the imaginary part. Taking the real part of both sides of this equation, using Eq. (S16), gives the single-sided representation of the homogeneous Green's function

$$
\begin{equation*}
G_{\mathrm{h}}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=\int_{\mathrm{S}_{0}} \frac{2}{\omega \rho(\boldsymbol{x})}\left(\left\{\partial_{i} G_{\mathrm{h}}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\right\} \Im\left\{f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}-G_{\mathrm{h}}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \Im\left\{\partial_{i} f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}\right) n_{i} \mathrm{~d} \boldsymbol{x} . \tag{S28}
\end{equation*}
$$

## S2.3 Single-sided homogeneous Green's function representation: assuming a homogeneous upper half-space

From here onward we assume that also $\mathbb{S}_{0}$ is a horizontal surface, with $\boldsymbol{n}=(0,0,-1)$. Substituting Eqs. (A39) and (A40) for the surface integrals at $\mathbb{S}_{0}$ and Eqs. (A47) and (A48) for the volume integrals into Eqs. (S20) and (S21), we obtain

$$
\begin{align*}
& \int_{\mathbb{V}_{\mathrm{A}}}\left(p_{\mathrm{A}}^{+} q_{\mathrm{B}}^{-}+p_{\mathrm{A}}^{-} q_{\mathrm{B}}^{+}-q_{\mathrm{A}}^{+} p_{\mathrm{B}}^{-}-q_{\mathrm{A}}^{-} p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x}= \\
& \qquad \int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right) p_{\mathrm{B}}^{-}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right) p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x}-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right) p_{\mathrm{B}}^{-}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right) p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{S29}
\end{align*}
$$

and, ignoring evanescent waves,

$$
\begin{align*}
& \int_{\mathbb{V}_{\mathrm{A}}}\left(p_{\mathrm{A}}^{+*} q_{\mathrm{B}}^{+}+p_{\mathrm{A}}^{-*} q_{\mathrm{B}}^{-}+q_{\mathrm{A}}^{+*} p_{\mathrm{B}}^{+}+q_{\mathrm{A}}^{-*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x}= \\
& \qquad \int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right)^{*} p_{\mathrm{B}}^{+}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right)^{*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x}-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right)^{*} p_{\mathrm{B}}^{+}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right)^{*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} . \tag{S30}
\end{align*}
$$

We apply these theorems to the situation in which the upper half-space above $\mathbb{S}_{0}$ is homogeneous (for the Green's function as well as for the focusing function). For state A we consider again the focusing function $f_{1}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+$ $f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)$, defined in a truncated version of the medium. For state B we consider the Green's function $G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)=$ $G^{+,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+G^{-,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+G^{+,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+G^{-,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$, with its source at $\boldsymbol{x}_{\mathrm{B}}$ anywhere in the half-space below $\mathbb{S}_{0}$. Note that we introduced two superscripts. The first superscript refers again to the propagation direction at the observation point $\boldsymbol{x}$. The second superscript refers to the radiation direction of the source at $\boldsymbol{x}_{\mathrm{B}}$. Substituting $q_{\mathrm{A}}^{+}(\boldsymbol{x}, \omega)=q_{\mathrm{A}}^{-}(\boldsymbol{x}, \omega)=0$, $p_{\mathrm{A}}^{ \pm}(\boldsymbol{x}, \omega)=f_{1}^{ \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right), q_{\mathrm{B}}^{+}(\boldsymbol{x}, \omega)=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right), q_{\mathrm{B}}^{-}(\boldsymbol{x}, \omega)=0$ and $p_{\mathrm{B}}^{ \pm}(\boldsymbol{x}, \omega)=G^{ \pm,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$ into Eqs. (S29) and (S30), using Eqs. (S22) and (S23) and $G^{+,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)=0$ for $\boldsymbol{x}$ at $\mathbb{S}_{0}$ (since the upper half-space is homogeneous), gives

$$
\begin{equation*}
G^{-,+}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+\chi\left(\boldsymbol{x}_{\mathrm{B}}\right) f_{1}^{-}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho_{0}} G^{-,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{3} f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right) \mathrm{d} \boldsymbol{x} \tag{S31}
\end{equation*}
$$

and

$$
\begin{equation*}
G^{+,+}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)-\chi\left(\boldsymbol{x}_{\mathrm{B}}\right)\left\{f_{1}^{+}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}^{*}=-\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho_{0}} G^{-,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\left\{\partial_{3} f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}^{*} \mathrm{~d} \boldsymbol{x} \tag{S32}
\end{equation*}
$$

Next, substituting $q_{\mathrm{A}}^{+}(\boldsymbol{x}, \omega)=q_{\mathrm{A}}^{-}(\boldsymbol{x}, \omega)=0, p_{\mathrm{A}}^{ \pm}(\boldsymbol{x}, \omega)=f_{1}^{ \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right), q_{\mathrm{B}}^{+}(\boldsymbol{x}, \omega)=0, q_{\mathrm{B}}^{-}(\boldsymbol{x}, \omega)=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right)$ and $p_{\mathrm{B}}^{ \pm}(\boldsymbol{x}, \omega)=$ $G^{ \pm,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$ into Eqs. (S29) and (S30), using Eqs. (S22) and (S23) and $G^{+,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)=0$ for $\boldsymbol{x}$ at $\mathbb{S}_{0}$, gives

$$
\begin{equation*}
G^{-,-}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)+\chi\left(\boldsymbol{x}_{\mathrm{B}}\right) f_{1}^{+}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho_{0}} G^{-,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{3} f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right) \mathrm{d} \boldsymbol{x} \tag{S33}
\end{equation*}
$$

and

$$
\begin{equation*}
G^{+,-}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)-\chi\left(\boldsymbol{x}_{\mathrm{B}}\right)\left\{f_{1}^{-}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}^{*}=-\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho_{0}} G^{-,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)\left\{\partial_{3} f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}^{*} \mathrm{~d} \boldsymbol{x} \tag{S34}
\end{equation*}
$$

Summing Eqs. (S31) - (S34), using source-receiver reciprocity for the Green's function on the left-hand side and $G^{+,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)=G^{+,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)=0$ for $\boldsymbol{x}$ at $\mathbb{S}_{0}$, we obtain

$$
\begin{align*}
& G\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+\chi\left(\boldsymbol{x}_{\mathrm{B}}\right) 2 i \Im\left\{f_{1}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\} \\
& \quad=\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho_{0}} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{3}\left(f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)-\left\{f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}^{*}\right) \mathrm{d} \boldsymbol{x} \tag{S35}
\end{align*}
$$

Taking the real part of both sides gives the single-sided representation of the homogeneous Green's function for the situation that the upper half-space is homogeneous

$$
\begin{equation*}
G_{\mathrm{h}}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=4 \Re \int_{\mathbb{S}_{0}} \frac{1}{i \omega \rho_{0}} G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \partial_{3}\left(f_{1}^{+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)-\left\{f_{1}^{-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)\right\}^{*}\right) \mathrm{d} \boldsymbol{x} \tag{S36}
\end{equation*}
$$

We conclude by deriving source-receiver reciprocity relations for the decomposed Green's functions $G^{ \pm, \pm}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$. We consider Eq. (S29), but replace $\mathbb{V}_{\mathrm{A}}$ by the entire space $\mathbb{R}^{3}$. In this situation there are only outgoing waves at $\mathbb{S}$. Hence, Eq. (S29) simplifies to

$$
\begin{equation*}
\int_{\mathbb{R}^{3}}\left(p_{\mathrm{A}}^{+} q_{\mathrm{B}}^{-}+p_{\mathrm{A}}^{-} q_{\mathrm{B}}^{+}-q_{\mathrm{A}}^{+} p_{\mathrm{B}}^{-}-q_{\mathrm{A}}^{-} p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x}=0 \tag{S37}
\end{equation*}
$$

First we substitute $q_{\mathrm{A}}^{+}=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{A}}\right), q_{\mathrm{A}}^{-}=0, p_{\mathrm{A}}^{ \pm}=G^{ \pm,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right), q_{\mathrm{B}}^{+}=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right), q_{\mathrm{B}}^{-}=0$ and $p_{\mathrm{B}}^{ \pm}=G^{ \pm,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$. This gives

$$
\begin{equation*}
G^{-,+}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=G^{-,+}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) \tag{S38}
\end{equation*}
$$

Next, we substitute $q_{\mathrm{A}}^{+}=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{A}}\right), q_{\mathrm{A}}^{-}=0, p_{\mathrm{A}}^{ \pm}=G^{ \pm,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right), q_{\mathrm{B}}^{+}=0, q_{\mathrm{B}}^{-}=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right)$ and $p_{\mathrm{B}}^{ \pm}=G^{ \pm,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$. This gives

$$
\begin{equation*}
G^{+,+}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=G^{-,-}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) . \tag{S39}
\end{equation*}
$$

Finally, we substitute $q_{\mathrm{A}}^{+}=0, q_{\mathrm{A}}^{-}=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{A}}\right), p_{\mathrm{A}}^{ \pm}=G^{ \pm,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right), q_{\mathrm{B}}^{+}=0, q_{\mathrm{B}}^{-}=\delta\left(\boldsymbol{x}-\boldsymbol{x}_{\mathrm{B}}\right)$ and $p_{\mathrm{B}}^{ \pm}=G^{ \pm,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{B}}, \omega\right)$. This gives

$$
\begin{equation*}
G^{+,-}\left(\boldsymbol{x}_{\mathrm{B}}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=G^{+,-}\left(\boldsymbol{x}_{\mathrm{A}}, \boldsymbol{x}_{\mathrm{B}}, \omega\right) . \tag{S40}
\end{equation*}
$$

Note that Eq. (S39) does not include a minus sign, unlike the corresponding relation for the flux-normalised decomposed Green's functions (Wapenaar, 1996a). This is due to the definition of $q^{ \pm}$in Eq. (A46). As a result of this definition, we have the following simple expression for the full Green's function

$$
\begin{equation*}
G\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)=G^{+,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+G^{-,+}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+G^{+,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right)+G^{-,-}\left(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{A}}, \omega\right) . \tag{S41}
\end{equation*}
$$

## Appendix A: Decomposition of the integrals in the reciprocity theorems

## A1 Matrix-vector wave equation

By eliminating $v_{1}$ and $v_{2}$ from Eqs. (S9) and (S10), we obtain the following matrix-vector wave equation in the space-frequency domain

$$
\begin{equation*}
\partial_{3} \boldsymbol{q}=\mathbf{A} \boldsymbol{q}+\boldsymbol{d}, \tag{A1}
\end{equation*}
$$

where

$$
\boldsymbol{q}=\binom{p}{v_{3}}, \quad \boldsymbol{d}=\binom{0}{q}, \quad \mathbf{A}=\left(\begin{array}{cc}
0 & \mathcal{A}_{12}  \tag{A2}\\
\mathcal{A}_{21} & 0
\end{array}\right),
$$

with

$$
\begin{align*}
& \mathcal{A}_{12}=i \omega \rho,  \tag{A3}\\
& \mathcal{A}_{21}=i \omega \kappa-\frac{1}{i \omega} \partial_{\alpha} \frac{1}{\rho} \partial_{\alpha} \tag{A4}
\end{align*}
$$

(Corones, 1975; Ursin, 1983; Fishman and McCoy, 1984; Wapenaar and Berkhout, 1989; de Hoop, 1996). Here $\partial_{\alpha}$ stands for the spatial differential operator $\partial / \partial x_{\alpha}$. Greek subscripts take on the values 1 and 2 and Einstein's summation convention applies to repeated subscripts. The notation in the right-hand side of Eq. (A4) should be understood in the sense that differential operators act on all factors to the right of it. Hence, operator $\partial_{\alpha} \frac{1}{\rho} \partial_{\alpha}$, applied via Eq. (A1) to $p$, stands for $\partial_{\alpha}\left(\frac{1}{\rho} \partial_{\alpha} p\right)$.

## A2 Decomposition of the matrix-vector wave equation

For the decomposition of the matrix-vector wave equation, we first recast the operator matrix $\mathbf{A}$ into a more symmetric form. To this end we define an operator $\mathcal{H}_{2}$, according to

$$
\begin{equation*}
\mathcal{H}_{2}=-i \omega \sqrt{\rho} \mathcal{A}_{21} \sqrt{\rho}=k^{2}+\sqrt{\rho} \partial_{\alpha} \frac{1}{\rho} \partial_{\alpha} \sqrt{\rho}, \tag{A5}
\end{equation*}
$$

with

$$
\begin{equation*}
k^{2}=\frac{\omega^{2}}{c^{2}}, \quad c=\frac{1}{\sqrt{\rho \kappa}} . \tag{A6}
\end{equation*}
$$

After some bookkeeping it follows that $\mathcal{H}_{2}$ can be written as a 2D Helmholtz operator

$$
\begin{equation*}
\mathcal{H}_{2}=k_{\mathrm{S}}^{2}+\partial_{\alpha} \partial_{\alpha} \tag{A7}
\end{equation*}
$$

(Wapenaar and Berkhout, 1989; de Hoop, 1992), with the scaled wavenumber $k_{\mathrm{S}}$ obeying

$$
\begin{equation*}
k_{\mathrm{S}}^{2}=\frac{\omega^{2}}{c^{2}}-\frac{3\left(\partial_{\alpha} \rho\right)\left(\partial_{\alpha} \rho\right)}{4 \rho^{2}}+\frac{\left(\partial_{\alpha} \partial_{\alpha} \rho\right)}{2 \rho} \tag{A8}
\end{equation*}
$$

(Brekhovskikh, 1960). We now rewrite operator matrix A as

$$
\mathbf{A}=\left(\begin{array}{cc}
0 & i \omega \rho  \tag{A9}\\
-\frac{1}{i \omega \sqrt{\rho}} \mathcal{H}_{2} \frac{1}{\sqrt{\rho}} & 0
\end{array}\right)
$$

The decomposition of this matrix is not unique. Flux-normalized decomposition is discussed by de Hoop (1996) and Wapenaar (1996b). Here we discuss a symmetric form of pressure-normalized decomposition, modified after Wapenaar and Berkhout (1989). We decompose the matrix as follows

$$
\begin{equation*}
\mathbf{A}=\mathbf{L} \mathbf{H L} \mathbf{L}^{-1} \tag{A10}
\end{equation*}
$$

with

$$
\mathbf{L}=\left(\begin{array}{cc}
1 & 1  \tag{A11}\\
\frac{1}{\omega \rho} \mathcal{H}_{1}^{s} & -\frac{1}{\omega \rho} \mathcal{H}_{1}^{s}
\end{array}\right), \quad \mathbf{H}=\left(\begin{array}{cc}
i \mathcal{H}_{1}^{s} & 0 \\
0 & -i \mathcal{H}_{1}^{s}
\end{array}\right), \quad \mathbf{L}^{-1}=\frac{1}{2}\left(\begin{array}{cc}
1 & \left(\frac{1}{\omega \rho} \mathcal{H}_{1}^{s}\right)^{-1} \\
1 & -\left(\frac{1}{\omega \rho} \mathcal{H}_{1}^{s}\right)^{-1}
\end{array}\right)
$$

Here

$$
\begin{equation*}
\mathcal{H}_{1}^{s}=\sqrt{\rho} \mathcal{H}_{1} \frac{1}{\sqrt{\rho}} \tag{A12}
\end{equation*}
$$

where $\mathcal{H}_{1}$ is the square-root of the Helmholtz operator, according to

$$
\begin{equation*}
\mathcal{H}_{1} \mathcal{H}_{1}=\mathcal{H}_{2} \tag{A13}
\end{equation*}
$$

We decompose the wave vector $\boldsymbol{q}$ and the source vector $\boldsymbol{d}$ as follows

$$
\begin{array}{ll}
\boldsymbol{q}=\mathbf{L} \boldsymbol{p}, & \boldsymbol{p}=\mathbf{L}^{-1} \boldsymbol{q} \\
\boldsymbol{d}=\mathbf{L} \boldsymbol{s}, & \boldsymbol{s}=\mathbf{L}^{-1} \boldsymbol{d} \tag{A15}
\end{array}
$$

with

$$
\begin{equation*}
\boldsymbol{p}=\binom{p^{+}}{p^{-}}, \quad \boldsymbol{s}=\binom{s^{+}}{s^{-}} \tag{A16}
\end{equation*}
$$

Substitution of Eqs. (A14) and (A15) into the matrix-vector wave equation (A1), using Eq. (A10), yields

$$
\begin{equation*}
\partial_{3} \boldsymbol{p}=\mathbf{B} \boldsymbol{p}+\boldsymbol{s} \tag{A17}
\end{equation*}
$$

with

$$
\begin{equation*}
\mathbf{B}=\mathbf{H}-\mathbf{L}^{-1} \partial_{3} \mathbf{L} \tag{A18}
\end{equation*}
$$

or

$$
\partial_{3}\binom{p^{+}}{p^{-}}=\left(\begin{array}{cc}
i \mathcal{H}_{1}^{s} & 0  \tag{A19}\\
0 & -i \mathcal{H}_{1}^{s}
\end{array}\right)\binom{p^{+}}{p^{-}}-\frac{1}{2}\left(\begin{array}{cc}
\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{-1} \partial_{3}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) & -\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{-1} \partial_{3}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) \\
-\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{-1} \partial_{3}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) & \left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{-1} \partial_{3}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)
\end{array}\right)\binom{p^{+}}{p^{-}}+\binom{s^{+}}{s^{-}}
$$

This is a system of coupled one-way wave equations for downgoing and upgoing waves, $p^{+}$and $p^{-}$, respectively. With the definitions of $\boldsymbol{q}$ and $\boldsymbol{p}$ in Eqs. (A2) and (A16), respectively, and $\mathbf{L}$ in Eq. (A11), it follows from Eq. (A14) that

$$
\begin{equation*}
p=p^{+}+p^{-} \tag{A20}
\end{equation*}
$$

Hence, the decomposed fields $p^{+}$and $p^{-}$are indeed pressure-normalised downgoing and upgoing waves.

## A3 Symmetry properties of the operators

For an operator $\mathcal{U}$, containing space-dependent medium parameters and differential operators $\partial_{1}$ and $\partial_{2}$, we introduce its transpose $\mathcal{U}^{t}$ and its adjoint (i.e., complex conjugate transpose) $\mathcal{U}^{\dagger}$ via
$\int_{\mathbb{A}}(\mathcal{U} f)^{t} g \mathrm{~d} \boldsymbol{x}=\int_{\mathbb{A}} f\left(\mathcal{U}^{t} g\right) \mathrm{d} \boldsymbol{x}$
and
$\int_{\mathbb{A}}(\mathcal{U} f)^{*} g \mathrm{~d} \boldsymbol{x}=\int_{\mathbb{A}} f^{*}\left(\mathcal{U}^{\dagger} g\right) \mathrm{d} \boldsymbol{x}$,
where $\mathbb{A}$ is an infinite horizontal integration surface at arbitrary depth $x_{3}$, and $f(\boldsymbol{x})$ and $g(\boldsymbol{x})$ are space-dependent functions with sufficient decay along $\mathbb{A}$ towards infinity. For the Helmholtz operator $\mathcal{H}_{2}$, defined in Eq. (A7), we have

$$
\begin{equation*}
\mathcal{H}_{2}^{t}=\mathcal{H}_{2}, \tag{A23}
\end{equation*}
$$

meaning $\mathcal{H}_{2}$ is a symmetric operator. Since we consider a lossless medium, we also have

$$
\begin{equation*}
\mathcal{H}_{2}^{\dagger}=\mathcal{H}_{2}^{*}=\mathcal{H}_{2}, \tag{A24}
\end{equation*}
$$

meaning $\mathcal{H}_{2}$ is also a self-adjoint operator.
The square-root operator $\mathcal{H}_{1}$, defined in Eq. (A13), is a pseudo-differential operator. It obeys the following symmetry property

$$
\begin{equation*}
\mathcal{H}_{1}^{t}=\mathcal{H}_{1}, \tag{A25}
\end{equation*}
$$

meaning $\mathcal{H}_{1}$ is a symmetric operator (Wapenaar and Grimbergen, 1996). Ignoring evanescent waves, we have

$$
\begin{equation*}
\mathcal{H}_{1}^{\dagger}=\mathcal{H}_{1}^{*} \approx \mathcal{H}_{1} . \tag{A26}
\end{equation*}
$$

Hence, this operator is not self-adjoint. In the following we replace approximation signs by equal signs whenever the only approximation is the negligence of evanescent waves. Operator $\mathcal{H}_{1}^{s}$, defined in Eq. (A12), obeys the following symmetry properties

$$
\begin{align*}
& \left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t}=\frac{1}{\rho} \mathcal{H}_{1}^{s},  \tag{A27}\\
& \left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger}=\frac{1}{\rho} \mathcal{H}_{1}^{s} . \tag{A28}
\end{align*}
$$

From these symmetry relations, we find that $\mathbf{L}$, defined in Eq. (A11), obeys the following properties

$$
\mathbf{L}^{t} \mathbf{N L}=\left(\begin{array}{cc}
0 & -\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)  \tag{A29}\\
\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) & 0
\end{array}\right)=\left(\begin{array}{cc}
0 & -\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t} \\
\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t} & 0
\end{array}\right)
$$

and, ignoring evanescent waves,

$$
\mathbf{L}^{\dagger} \mathbf{K} \mathbf{L}=\left(\begin{array}{cc}
\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) & 0  \tag{A30}\\
0 & -\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)
\end{array}\right)=\left(\begin{array}{cc}
\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger} & 0 \\
0 & -\frac{2}{\omega}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger}
\end{array}\right),
$$

with

$$
\mathbf{N}=\left(\begin{array}{cc}
0 & 1  \tag{A31}\\
-1 & 0
\end{array}\right), \quad \mathbf{K}=\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right) .
$$

## A4 Decomposition of the surface integrals

For the surface integrals along $\mathbb{S}_{\mathrm{A}}$ appearing in Eqs. (S18) and (S19) we introduce the following compact notation (using $\frac{1}{i \omega \rho} \partial_{3} p=v_{3}$ )

$$
\begin{equation*}
\int_{\mathbb{S}_{\mathrm{A}}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{\mathrm{A}}} \boldsymbol{q}_{\mathrm{A}}^{t} \mathbf{N} \boldsymbol{q}_{\mathrm{B}} \mathrm{~d} \boldsymbol{x} \tag{A32}
\end{equation*}
$$

and

$$
\begin{equation*}
\int_{\mathbb{S}_{\mathrm{A}}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}^{*}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{\mathrm{A}}} \boldsymbol{q}_{\mathrm{A}}^{\dagger} \mathbf{K} \boldsymbol{q}_{\mathrm{B}} \mathrm{~d} \boldsymbol{x} \tag{A33}
\end{equation*}
$$

respectively. With the decomposition of $\boldsymbol{q}$ defined in Eq. (A14), the properties of $\mathbf{L}$ formulated in Eqs. (A29) and (A30), and the definition of $\boldsymbol{p}$ in Eq. (A16) we obtain

$$
\begin{equation*}
\int_{\mathbb{S}_{\mathrm{A}}} \boldsymbol{q}_{\mathrm{A}}^{t} \mathbf{N} \boldsymbol{q}_{\mathrm{B}} \mathrm{~d} \boldsymbol{x}=\int_{\mathbb{S}_{\mathrm{A}}} \boldsymbol{p}_{\mathrm{A}}^{t} \mathbf{L}^{t} \mathbf{N L} \boldsymbol{p}_{\mathrm{B}} \mathrm{~d} \boldsymbol{x}=-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{\omega}\left(p_{\mathrm{A}}^{+}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t} p_{\mathrm{B}}^{-}-p_{\mathrm{A}}^{-}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t} p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{A34}
\end{equation*}
$$

and, ignoring evanescent waves,

$$
\begin{equation*}
\int_{\mathbb{S}_{\mathrm{A}}} \boldsymbol{q}_{\mathrm{A}}^{\dagger} \mathbf{K} \boldsymbol{q}_{\mathrm{B}} \mathrm{~d} \boldsymbol{x}=\int_{\mathbb{S}_{\mathrm{A}}} \boldsymbol{p}_{\mathrm{A}}^{\dagger} \mathbf{L}^{\dagger} \mathbf{K} \mathbf{L} \boldsymbol{p}_{\mathrm{B}} \mathrm{~d} \boldsymbol{x}=\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{\omega}\left(p_{\mathrm{A}}^{+*}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger} p_{\mathrm{B}}^{+}-p_{\mathrm{A}}^{-*}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} \tag{A35}
\end{equation*}
$$

Assuming that in state $A$ there are no vertical derivatives of the medium parameters at $\mathbb{S}_{A}$, we find from Eq. (A19)

$$
\begin{equation*}
\partial_{3} p_{\mathrm{A}}^{ \pm}= \pm i \mathcal{H}_{1}^{s} p_{\mathrm{A}}^{ \pm} \quad \text { at } \mathbb{S}_{\mathrm{A}} . \tag{A36}
\end{equation*}
$$

Using this in Eqs. (A34) and (A35) and substituting the results into Eqs. (A32) and (A33), we obtain

$$
\begin{equation*}
\int_{\mathbb{S}_{\mathrm{A}}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right) p_{\mathrm{B}}^{-}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right) p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{A37}
\end{equation*}
$$

and, ignoring evanescent waves,

$$
\begin{equation*}
\int_{\mathbb{S}_{\mathrm{A}}} \frac{1}{i \omega \rho}\left\{p_{\mathrm{A}}^{*}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=-\int_{\mathbb{S}_{\mathrm{A}}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right)^{*} p_{\mathrm{B}}^{+}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right)^{*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} \tag{A38}
\end{equation*}
$$

When $\mathbb{S}_{0}$ in Eqs. (S18) and (S19) is also a horizontal surface, with $\boldsymbol{n}=(0,0,-1)$, we obtain (assuming that in state A there are no vertical derivatives of the medium parameters at $\mathbb{S}_{0}$ )

$$
\begin{equation*}
\int_{\mathbb{S}_{0}} \frac{-1}{i \omega \rho}\left\{p_{\mathrm{A}}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right) p_{\mathrm{B}}^{-}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right) p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{A39}
\end{equation*}
$$

and, ignoring evanescent waves,

$$
\begin{equation*}
\int_{\mathbb{S}_{0}} \frac{-1}{i \omega \rho}\left\{p_{\mathrm{A}}^{*}\left(\partial_{3} p_{\mathrm{B}}\right)-\left(\partial_{3} p_{\mathrm{A}}^{*}\right) p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{S}_{0}} \frac{2}{i \omega \rho}\left(\left(\partial_{3} p_{\mathrm{A}}^{+}\right)^{*} p_{\mathrm{B}}^{+}+\left(\partial_{3} p_{\mathrm{A}}^{-}\right)^{*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} . \tag{A40}
\end{equation*}
$$

## A5 Decomposition of the volume integrals

Assuming both $\mathbb{S}_{0}$ and $\mathbb{S}_{\mathrm{A}}$ are horizontal surfaces, we introduce the following compact notation for the volume integrals in Eqs. (S18) and (S19)

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left\{p_{\mathrm{A}} q_{\mathrm{B}}-q_{\mathrm{A}} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{V}_{\mathrm{A}}}\left(\boldsymbol{d}_{\mathrm{A}}^{t} \mathbf{N} \boldsymbol{q}_{\mathrm{B}}+\boldsymbol{q}_{\mathrm{A}}^{t} \mathbf{N} \boldsymbol{d}_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x} \tag{A41}
\end{equation*}
$$

and

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left\{p_{\mathrm{A}}^{*} q_{\mathrm{B}}+q_{\mathrm{A}}^{*} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{V}_{\mathrm{A}}}\left(\boldsymbol{d}_{\mathrm{A}}^{\dagger} \mathbf{K} \boldsymbol{q}_{\mathrm{B}}+\boldsymbol{q}_{\mathrm{A}}^{\dagger} \mathbf{K} \boldsymbol{d}_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x} \tag{A42}
\end{equation*}
$$

respectively. With the decomposition of $\boldsymbol{q}$ and $\boldsymbol{d}$ defined in Eqs. (A14) and (A15), the properties of $\mathbf{L}$ formulated in Eqs. (A29) and (A30), and the definition of $\boldsymbol{p}$ and $\boldsymbol{s}$ in Eq. (A16), we obtain

$$
\begin{align*}
& \int_{\mathbb{V}_{\mathrm{A}}}\left(\boldsymbol{d}_{\mathrm{A}}^{t} \mathbf{N} \boldsymbol{q}_{\mathrm{B}}+\boldsymbol{q}_{\mathrm{A}}^{t} \mathbf{N} \boldsymbol{d}_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x}=\int_{\mathbb{V}_{\mathrm{A}}}\left(\boldsymbol{s}_{\mathrm{A}}^{t} \mathbf{L}^{t} \mathbf{N L} \boldsymbol{p}_{\mathrm{B}}+\boldsymbol{p}_{\mathrm{A}}^{t} \mathbf{L}^{t} \mathbf{N L} \boldsymbol{s}_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x} \\
& =-\int_{\mathbb{V}_{\mathrm{A}}} \frac{2}{\omega}\left(s_{\mathrm{A}}^{+}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t} p_{\mathrm{B}}^{-}-s_{\mathrm{A}}^{-}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{t} p_{\mathrm{B}}^{+}+p_{\mathrm{A}}^{+}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) s_{\mathrm{B}}^{-}-p_{\mathrm{A}}^{-}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) s_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{A43}
\end{align*}
$$

and, ignoring evanescent waves,

$$
\begin{align*}
& \int_{\mathbb{V}_{\mathrm{A}}}\left(\boldsymbol{d}_{\mathrm{A}}^{\dagger} \mathbf{K} \boldsymbol{q}_{\mathrm{B}}+\boldsymbol{q}_{\mathrm{A}}^{\dagger} \mathbf{K} \boldsymbol{d}_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x}=\int_{\mathbb{V}_{\mathrm{A}}}\left(\boldsymbol{s}_{\mathrm{A}}^{\dagger} \mathbf{L}^{\dagger} \mathbf{K} \mathbf{L} \boldsymbol{p}_{\mathrm{B}}+\boldsymbol{p}_{\mathrm{A}}^{\dagger} \mathbf{L}^{\dagger} \mathbf{K} \mathbf{L} \boldsymbol{s}_{\mathrm{B}}\right) \mathrm{d} \boldsymbol{x} \\
& =\int_{\mathbb{V}_{\mathrm{A}}} \frac{2}{\omega}\left(s_{\mathrm{A}}^{+*}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger} p_{\mathrm{B}}^{+}-s_{\mathrm{A}}^{-*}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right)^{\dagger} p_{\mathrm{B}}^{-}+p_{\mathrm{A}}^{+*}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) s_{\mathrm{B}}^{+}-p_{\mathrm{A}}^{-*}\left(\frac{1}{\rho} \mathcal{H}_{1}^{s}\right) s_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} . \tag{A44}
\end{align*}
$$

From $\boldsymbol{s}=\mathbf{L}^{-1} \boldsymbol{d}$, and the definitions of $\boldsymbol{d}, \mathbf{L}^{-1}$ and $\boldsymbol{s}$ in Eqs. (A2), (A11) and (A16), we find

$$
\begin{equation*}
s^{ \pm}= \pm\left(\frac{2}{\omega \rho} \mathcal{H}_{1}^{s}\right)^{-1} q \tag{A45}
\end{equation*}
$$

We define new decomposed sources $q^{+}$and $q^{-}$, according to

$$
\begin{equation*}
q^{ \pm}= \pm \frac{2}{\omega \rho} \mathcal{H}_{1}^{s} s^{ \pm} \tag{A46}
\end{equation*}
$$

Using this definition in Eqs. (A43) and (A44) and substituting the results in Eqs. (A41) and (A42), we obtain

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left\{p_{\mathrm{A}} q_{\mathrm{B}}-q_{\mathrm{A}} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{V}_{\mathrm{A}}}\left(p_{\mathrm{A}}^{+} q_{\mathrm{B}}^{-}+p_{\mathrm{A}}^{-} q_{\mathrm{B}}^{+}-q_{\mathrm{A}}^{+} p_{\mathrm{B}}^{-}-q_{\mathrm{A}}^{-} p_{\mathrm{B}}^{+}\right) \mathrm{d} \boldsymbol{x} \tag{A47}
\end{equation*}
$$

and, ignoring evanescent waves,

$$
\begin{equation*}
\int_{\mathbb{V}_{\mathrm{A}}}\left\{p_{\mathrm{A}}^{*} q_{\mathrm{B}}+q_{\mathrm{A}}^{*} p_{\mathrm{B}}\right\} \mathrm{d} \boldsymbol{x}=\int_{\mathbb{V}_{\mathrm{A}}}\left(p_{\mathrm{A}}^{+*} q_{\mathrm{B}}^{+}+p_{\mathrm{A}}^{-*} q_{\mathrm{B}}^{-}+q_{\mathrm{A}}^{+*} p_{\mathrm{B}}^{+}+q_{\mathrm{A}}^{-*} p_{\mathrm{B}}^{-}\right) \mathrm{d} \boldsymbol{x} \tag{A48}
\end{equation*}
$$

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