Monte Carlo simulations of coupled body- and Rayleigh-wave multiple scattering in elastic media

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SUMMARY

Seismic coda waves are commonly used in estimation of subsurface Q values and monitoring subsurface changes. Coda waves mainly consist of multiply scattered body and surface waves. These two types of waves interact with each other in the multiple scattering process, which thus leads to a spatiotemporal evolution of the body- and surface-wave energies. One cannot characterize the evolution because one has not fully understood the multiple scattering of the two types of waves. Thus one commonly assumes only one type of waves exists or ignores their interaction while studying the coda waves. However, neglecting the interaction leads to an incorrect energy evolution of the two types of waves and consequently biases the Q estimation or interpretation of coda-wave changes for monitoring. To better understand the interaction between these waves during multiple scattering and to model the energy evolution correctly, we propose a Monte Carlo algorithm to model the multiple scattering process. We describe the physics of the scattering for the two types of waves and derive scattering properties like cross sections for perturbations in elastic properties (e.g. density, shear modulus and Lamé parameters). Our algorithm

incorporates this knowledge and thus physically models the body- and surface-wave energy evolution in space and time. The energy partitioning ratios between surface and body waves provided by our algorithm match the theoretical prediction based on equipartition theory. In the equipartition state, our simulation results also match Lambert’s cosine law for body waves on the free surface. We discuss how the Rayleigh-to-body-wave scattering affects the energy partitioning ratios. Our algorithm provides a new tool to study multiple scattering and coda waves in elastic media with a free surface.

Key words: Wave scattering and diffraction; Coda waves; Computational seismology; Surface waves and free oscillations.

1 INTRODUCTION

Coda waves are arrivals after direct waves in seismic recordings or seismic crosscorrelations. One commonly uses coda waves to investigate and monitor the subsurface. By studying coda waves from an earthquake event, one can estimate subsurface Q values (e.g. Aki & Chouet 1975). One can also compare the coda waves in two event recordings and estimate differences in the coda-wave arrival times (e.g. Poupinet et al. 1984; Snieder et al. 2002; Mikesell et al. 2015) or waveforms (e.g. Larose et al. 2010). This method is called coda wave interferometry (CWI) monitoring. By assuming the two events share a similar source location and focal mechanism, one can qualitatively conclude that these differences are due to small changes of seismic properties (e.g. density) in the subsurface (e.g. Snieder 2006). This monitoring method has been applied to repeated event data in nature (e.g. Grêt et al. 2005) and in the lab (e.g. Larose et al. 2010). This method is also commonly applied to the coda waves in seismic crosscorrelations to monitor things such as the seasonal subsurface variations (e.g. Sens-Schönfelder & Wegler 2006; Wang et al. 2017), volcanic eruptions (e.g. Brenguier et al. 2007, 2008), ice sheet melting (e.g. Mordret et al. 2016) or the groundwater transport (e.g. Clements & Denolle 2018). One can further quantitatively image small changes in the subsurface from the CWI monitoring results (i.e. coda-wave differences) using the physics of coda waves (e.g. Pacheco & Snieder 2005; Planès et al. 2015; Margerin et al. 2016).

One routinely utilizes multiply scattered waves in the coda waves in both attenuation and CWI monitoring studies. *Multiply scattered* implies that these waves have scattered more than once in the subsurface while propagating from a (virtual) source to a receiver. In mod-

elling multiply scattered waves, one rarely uses wave equation solvers because the simulation requires so many simulation steps that both the computation cost and simulation result storage are prohibitively expensive. An alternative to the full-wavefield simulation is radiative transfer theory, which can be used to model the spatiotemporal evolution of the seismic wave energy/envelope (e.g. Wu 1985; Weaver 1990; Ryzhik et al. 1996). In the case of coupled elastic P and S waves, there exist semi-analytical solutions for the radiative transfer equations in homogeneous media (e.g. Zeng 1993; Sato 1994), given the scattered-wave amplitudes are isotropic. For inhomogeneous media and/or anisotropic scattering, one can adopt a Monte Carlo simulation approach to solve the radiative transfer equations numerically (e.g. Gusev & Abubakirov 1987; Hoshiya 1995, 1997). Furthermore, when using this approach, one only needs to know the properties of scattering (e.g. scattered-wave amplitudes and mean free paths) without explicitly referring to the radiative transfer equations (e.g. Margerin et al. 1998; Sanborn et al. 2017).

Most research on the radiative transfer theory so far has focused on either body or surface waves, but neglected the interaction between the two. However, both body and surface waves are present during the scattering process and they convert to one another via scattering (e.g. Maeda et al. 2008). Thus the energy ratio between the two types of waves evolves in time and space. Furthermore, Obermann et al. (2013) and Obermann et al. (2016) reveal that these two waves possess different sensitivities to subsurface elastic parameters through full wavefield simulations. Therefore, it is necessary to characterize the spatiotemporal evolution of the energy partitioning ratio between body and surface waves, so that one can estimate Q accurately or physically interpret the monitoring results (i.e. coda-wave differences). In current practice, one empirically assumes the energy ratios (e.g. Obermann et al. 2019) or ignores one of the two types of waves (e.g. Sens-Schönfelder & Wegler 2006; Mainsant et al. 2012; Obermann et al. 2015).

There have been previous attempts to incorporate the coupling between surface and body waves within a radiative transfer framework. To incorporate this coupling into the radiative transfer equations, Tregoures & Van Tiggelen (2002) considered body, Rayleigh, and Lamb waves in an elastic plate with a free surface boundary condition on each surface (top and bottom), where Rayleigh and Lamb waves are both a mixture of elastic body (P and S) waves; Borcea et al. (2021) approximated surface waves with acoustic waves trapped in a thin layer of an acoustic two-layer plate bounded by reflecting surfaces at the top and bottom. In both approaches the body waves cannot leak away at depth, which is not realistic for most Earth applications. Zeng (2006) introduced radiative transfer equations for coupled surface and body

waves by simplifying the coupling. However, these approximations and the simplification are hard to justify entirely from first principles. Margerin et al. (2019) extended the conventional radiative transfer equation by incorporating the coupling between surface and body waves in the context of the Helmholtz equation with an impedance-type boundary condition. As Margerin et al. (2019) used the scalar Helmholtz equation, only one type of body wave exists in their treatment. Based on the Born approximation, Margerin et al. (2019) derived the scattering mean free times for surface and body waves in a homogeneous velocity model with uniformly distributed point scatterers. Margerin et al. (2019) demonstrated that the surface-wave scattering properties (e.g. mean free time) depend on depth, and they used a Monte Carlo simulation to model the energy coupling between surface and body waves. However, a significant shortcoming is that different types of body (P and S) waves can not be incorporated into the simulation, because the simulation is based on the scalar equation. To overcome that limitation, we take advantage of Maeda et al. (2008) who theoretically described the scattering process between body and surface waves in detail. Based on these results, we derive key scattering properties (e.g. cross sections and mean free time/path, Section 2), and then we use these properties to develop a Monte Carlo simulation algorithm (e.g. Hoshioka 1991; Margerin et al. 2000) to model the body- and Rayleigh-wave multiple scattering process (Section 3). We focus on perturbations in density (ρ), where these perturbations ($\delta\rho$) act as scatterers in the media. One could extend our simulation algorithm to perturbations of P-wave and S-wave velocities using Birch's Law. We conduct the simulation with and without a P-S coupling free-surface boundary condition and then estimate the temporal energy ratios from multiply-scattered Rayleigh and body waves (Section 4). The temporal energy ratios eventually reach steady values, i.e. equipartition ratios. We verify the simulation by comparing the equipartition ratios to theoretical equipartition predictions. We finally discuss how to improve this algorithm (Section 5). Our algorithm can improve coda-wave studies about attenuation and the use of CWI for monitoring.

2 THE SCATTERING PROCESS

Knowledge of body- and Rayleigh-wave scattering processes is central for the radiative transfer theory and Monte Carlo simulations. For example, in an elastic medium, there is body wave to Rayleigh wave scattering denoted here as BR scattering. We consider three types of body waves: P, Sv and Sh waves. Thus we have three types of BR scattering: PR, SvR and ShR. Following the same logic, there is also Rayleigh wave to body wave (RB: RP/RSv/RSh), Rayleigh wave to Rayleigh wave (RR) and body wave to body wave (BB such as PP, PSv

and PSh) scattering. For all of these scattering cases, we present the single scattering cross sections (i.e. the ratio of scattered wave energy to the incident wave energy flux) and the multiply scattering mean free path/time (which indicates how efficiently the incident wave energy will be scattered). All the equations in this study are presented in the frequency domain. Different Fourier transform conventions do not affect our equations, because the conventions mainly impact the sign of phase while we focus on energy transport in this study.

2.1 Wave intensity

Wave intensity is normally used to measure the energy flux density of a wave, and the intensity is the base for calculating the wave scattering properties known as cross section and mean free path/time. The intensity of an incident P wave in a homogeneous medium is

$$I^P(\omega) = \rho_0 \alpha_0 \omega^2 |A^{0P}|^2, \quad (1)$$

where ρ_0 is the medium density, α_0 is the P-wave velocity, ω is the angular frequency and A^{0P} is the incident P-wave displacement amplitude (Aki & Richards 2002). The P-wave displacement amplitude is a function of frequency and we only focus on one frequency (i.e. ω) here. Similarly, the intensity of a S wave is

$$I^S(\omega) = \rho_0 \beta_0 \omega^2 |A^{0S}|^2, \quad (2)$$

where the S wave can be either Sv or Sh and β_0 is the S-wave velocity. We set the polarization direction for the incident Sh wave ($\mathbf{e}^{Sh}$) as the y-axis direction ($[0,1,0]$) in the following examples for simplicity (Figure 1). The units of I^P and I^S are both $J/(m^2s)$, where J represents the unit of energy, Joule.

The intensity of a Rayleigh wave is different from a body wave because a Rayleigh wave propagates along the surface with depth-dependent displacements. Thus the intensity of a Rayleigh wave is defined with a depth integral as (Aki & Richards 2002)

$$I^R(\omega) = \rho_0 U_R \omega^2 (A^{0R})^2 \int_0^\infty [r_1^2(z, \omega) + r_2^2(z, \omega)] dz, \quad (3)$$

where U_R is the Rayleigh-wave group velocity at the frequency ω , A^{0R} is the Rayleigh-wave amplitude, and r_1 and r_2 are the horizontal and vertical displacement eigenfunctions of the Rayleigh wave (Appendix A). The eigenfunctions vary with the depth and frequency. For brevity, we write this integral as $\int (r_1^2 + r_2^2) dz$. Notice that the units of $I^P(I^S)$ and I^R are $J/(m^2s)$ and $J/(ms)$, respectively. The unit difference is due to the depth integral. We demonstrate how this difference affects our analysis of Rayleigh-wave scattering in the following section.

Figure 1. An illustration of single scattering process. The block is the scatterer. The thin black arrows represent local coordinate system. The thick black arrows are body waves. The gray arrows are Rayleigh waves. The gray shapes below the gray arrows represent the Rayleigh-wave eigenfunctions which decrease with depth increasing.

2.2 Single scattering

The scattering cross section is defined for a single scattering, in which an incoming wave encounters a scatterer, as the ratio between the energy radiated by the scatterer in all outgoing propagation directions and the energy flux of the incoming wave. This ratio measures the efficacy of the single scattering process. In elastic media, we need to calculate the cross section for four types of single scattering: BR, RB, RR and BB. Calculation of each cross section requires the corresponding scattering amplitude (e.g. Margerin et al. 2000). We use the scattering amplitudes derived by Maeda et al. (2008) based on the Born approximation. We consider scattering related to Rayleigh waves as an example in this section.

2.2.1 BR scattering

The ShR indicates a scattered Rayleigh wave from an incident Sh wave and is an example of BR scattering. The m -component amplitude of a scattered Rayleigh wave due to a perturbation of density ($\delta\rho$) at $\mathbf{x}_s$ is

$$A_{m,\rho}^{ShR}(\mathbf{x}, \omega) = \int_V \sum_n G_{mn}(\mathbf{x}, \mathbf{x}_s, \omega) \omega^2 \delta\rho A_n^{0Sh} e_n^{Sh} d\mathbf{x}_s. \quad (4)$$

e_n^{Sh} is the n -component of incident Sh wave polarization vector, $[0,1,0]$ (Figure 1). Based on the Born approximation, the incident Sh wave scattering at $\delta\rho$ acts like a seismic source and generates scattered Rayleigh waves (e.g. Snieder 1986a; Maeda et al. 2008). Thus Equation 4 is a convolution between the Rayleigh-wave Green's function and a source term ($\omega^2 A_n^{0Sh} \delta\rho$). The amplitude of the far-field Rayleigh-wave Green's function is

$$G_{mn}(\mathbf{x}, \mathbf{x}_s, \omega) = \frac{p_m(z, \omega) p_n^*(z_s, \omega)}{4c_R U_R \int \rho_0 (r_1^2 + r_2^2) dz} \sqrt{\frac{2}{\pi k_R \Delta}}, \quad (5)$$

where $k_R = \omega/c_R$ and c_R is Rayleigh-wave phase velocity at frequency ω . p_m is a projection of the Rayleigh-wave eigenfunction (r_1 or r_2) in the m direction, like $[r_1 \cos \xi_1, r_1 \sin \xi_1, ir_2]$, where ξ_1 (Figure 1) is the scattered Rayleigh-wave propagation azimuth taken from the incident wave azimuth (Snieder 1986a; Maeda et al. 2008). Δ is the scattered Rayleigh-wave travel distance from $\mathbf{x}_s$ to $\mathbf{x}$ along Earth's surface. z_s is the depth of perturbation $\delta\rho$ and ρ_0 is the unperturbed/background density of the medium. The units of $\delta\rho$ and ρ_0 are both kg/m^3 . The scalar product between the polarization vectors in Equation 4 ($\sum_n p_n^* e_n^{0Sh}$) determines the coupling between the incident Sh and scattered Rayleigh waves. As the incident Sh wave only possesses a horizontal component in the y direction ($n = 2$), $\sum_n p_n^* e_n^{0Sh}$ becomes p_2^* , i.e. $r_1 \sin \xi_1$. We then rewrite Equation 4 as

$$A_{m,\rho}^{ShR}(\mathbf{x}, \omega) = A_n^{0Sh} \frac{\omega^2 p_m(z, \omega)}{4c_R U_R \int (r_1^2 + r_2^2) dz} \sqrt{\frac{2}{\pi k_R \Delta}} \int_V r_1(z_s, \omega) \sin \xi_1 \frac{\delta\rho}{\rho_0} d\mathbf{x}_s. \quad (6)$$

In Equation 6, we remark that the scattered Rayleigh-wave amplitude does not depend on the incident Sh wave angle (ψ_0). Instead, we observe that the Rayleigh-wave amplitude depends on the Rayleigh-wave propagation azimuth (ξ_1), and this observation offers physical insights into the scattering process. For example, if the scattered Rayleigh wave follows the same azimuth as the incident wave ($\xi_1 = 0$), we have $\sin \xi_1 = 0$ and as a consequence, the scattered amplitude is 0, which implies the absence of the ShR conversion in the forward direction. This result, sometimes termed as selection rule, fits our physical intuition. An incident Sh wave with particle motion in y direction does not excite a Rayleigh-wave propagating in x direction

because the two directions are orthogonal; furthermore, among all azimuths, the strongest excitation of Rayleigh waves occurs in the Sh wave polarization direction, i.e. the y direction.

We next assume that the size of the density perturbation is negligible compared to the Rayleigh-wave wavelength and further simplify Equation 6. Thus, we are in the so-called Rayleigh scattering regime (e.g. Wu & Aki 1985) and can rewrite Equation 6 as

$$A_{m,\rho}^{ShR}(\mathbf{x}, \omega) = A^{0Sh} \frac{\omega^2 p_m(z, \omega)}{4c_R U_R \int (r_1^2 + r_2^2) dz} \sqrt{\frac{2}{\pi k_R \Delta}} r_1(z_s, \omega) \sin \xi_1 V \frac{\delta \rho}{\rho_0}, \quad (7)$$

where we define $V = \int_V d\mathbf{x}_s$, the volume of a single scatterer. We then calculate the total energy of all the scattered Rayleigh waves by integrating the intensity over all azimuths using a cylindrical surface (S) integral:

$$E_\rho^{ShR}(z_s, \omega) = \rho_0 U_R \omega^2 \int_S \sum_m |A_{m,\rho}^{ShR}|^2 \Delta d\xi_1 dz, \quad (8)$$

$$= \rho_0 \omega^5 \frac{[A^{0Sh} r_1(z_s, \omega)]^2}{8c_R U_R \int (r_1^2 + r_2^2) dz} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (9)$$

where $A_{m,\rho}^{ShR}$ is from Equation 7 and $\int \sum_m |p_m|^2 dz / \int (r_1^2 + r_2^2) dz = 1$. We observe that the total energy depends on the scatterer depth, z_s . Based on the definition of the scattering cross section, we write the ShR cross section as

$$\sigma_\rho^{ShR}(z_s, \omega) = \frac{E_\rho^{ShR}}{I^{Sh}} = \frac{\omega^3}{8\beta_0 c_R U_R \int (r_1^2 + r_2^2) dz} r_1^2(z_s, \omega) V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2. \quad (10)$$

The unit for this cross section is m^2 . Notice this cross section depends explicitly on the scatterer depth (z_s) through the Rayleigh-wave eigenfunction, r_1 . Following the same logic, we write cross sections for the remaining BR and BB scattering in Appendix B. In contrast to the BR scattering, the BB cross sections are independent of the scatterer depth.

2.2.2 RB scattering

We next calculate the cross sections for incident Rayleigh waves. Following the same steps as above, for example, we can write the RSh cross section due to $\delta \rho$ as

$$\sigma_\rho^{RSh}(z_s, \omega) = \frac{E_\rho^{RSh}}{I^R} = \frac{\omega^4 r_1^2(z_s, \omega)}{8\pi \beta_0^3 U_R \int (r_1^2 + r_2^2) dz} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2. \quad (11)$$

Notice the unit for σ_ρ^{RSh} is m , instead of m^2 like σ_ρ^{ShR} . This is because of the unit difference between I^R and I^{Sh} (Section 2.1). For future reference, we introduce the following depth integrated cross section:

$$\bar{\sigma}_\rho^{RSh}(\omega) = \int_0^\infty \sigma_\rho^{RSh} dz_s = \frac{\omega^4 \int r_1^2(z_s, \omega) dz_s}{8\pi \beta_0^3 U_R \int (r_1^2 + r_2^2) dz} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (12)$$

where the cross section unit is m^2 . The definition is valid for a uniform and random distribution of point scatterers, where the scattering of Rayleigh waves is directly proportional to the depth integrated cross section. Following the same logic, we write the other RB and RR cross sections (Appendix B). Notice that, the averaged RB and averaged RR cross sections are both independent of the scatterer depth.

2.3 Isotropic incident angle assumption

Some cross sections are dependent on the incident angle, ψ_0 (Figure 1). For example, for a P wave scattered to a Rayleigh wave, the incident P-wave particle motion projects on both the x and z directions unless the P wave propagates purely vertically or horizontally. Thus σ_ρ^{PR} depends on the incident angle (ψ_0), and we derive the cross section by following the same steps as in Section 2.2:

$$\sigma_\rho^{PR} = \frac{\omega^3}{8\alpha_0 c_R U_R \int (r_1^2 + r_2^2) dz} (r_1^2 \sin^2 \psi_0 + 2r_2^2 \cos^2 \psi_0) V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2. \quad (13)$$

We observe that $\frac{\omega^3}{8\alpha_0 c_R U_R \int (r_1^2 + r_2^2) dz}$ is very similar to $\frac{\omega^3}{8\beta_0 c_R U_R \int (r_1^2 + r_2^2) dz}$ in ShR scattering (Equation 10) except the different incident wave velocities. We write $C = r_1^2 \sin^2 \psi_0 + 2r_2^2 \cos^2 \psi_0$ and note that this term, similar to r_1^2 in Equation 10, determines the coupling between the incident P and scattered Rayleigh waves. For example, $\psi_0 = 0$ (a vertically incident P-wave) and $\psi_0 = \pi/2$ (a horizontally incident P-wave) lead to purely vertical ($C = 2r_2^2$) and horizontal ($C = r_1^2$) coupling, respectively. Therefore the PR cross section dependence on ψ_0 makes intuitive sense. This phenomenon also exists in the SvR scattering (Appendix B).

Equation 13 explicitly indicates that the BR scattering involves the body-wave incident angle. This involvement significantly complicates any simulation, especially the following Monte Carlo simulation, because we need to calculate the BR cross section for a given incident angle (ψ_0) and use the new cross section to determine scattering Rayleigh-wave azimuths (ξ_1). Furthermore, numerical simulations (e.g. Paul et al. 2005) demonstrate that the incident angles become evenly distributed on the unit sphere (i.e. isotropic) after a sufficiently large number of scattering events. Thus, we can eliminate the incident angle dependence of the BR scattering cross sections (e.g. σ_ρ^{PR}) by averaging the cross sections over the incident angles (ψ_0):

$$\tilde{\sigma}_\rho^{PR} = \frac{1}{\int_0^\pi \sin \psi_0 d\psi_0} \int_0^\pi \sigma_\rho^{PR} \sin \psi_0 d\psi_0 = \frac{\omega^3}{12\alpha_0 c_R U_R \int (r_1^2 + r_2^2) dz} (r_1^2 + r_2^2) V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2. \quad (14)$$

Following the same process, we average other incident-angle dependent cross sections and present the results in Appendix B.

2.4 Multiple scattering

The knowledge of single scattering is the building block for multiple scattering, since multiple scattering can be modeled as a series of single scattering events in wave propagation from a (virtual) source to a receiver. This connection between multiple scattering and single scattering is known as the independent scattering approximation (e.g. Lagendijk & Van Tiggelen 1996). In the approximation, we define a volume density of point scatterers (n , unit: m^{-3}) and write the mean free path (l^w) for an incident wave as

$$l^w = \frac{1}{n\sigma^w}, \quad (15)$$

where σ^w is the sum of all the possible single-scattering cross sections for the incident wave (e.g. Margerin et al. 2000), such as $\sigma_\rho^{Sh}(z, \omega) = \sigma_\rho^{ShR}(z, \omega) + \sigma_\rho^{ShP}(\omega) + \sigma_\rho^{ShSv}(\omega) + \sigma_\rho^{ShSh}(\omega)$ in this study. The mean free path indicates the average distance between two scattering events (e.g. Hoshiba 1991) and has the unit of m . The mean free path also indicates the energy being scattered: a smaller mean free path means there will be more scattered wave energy in the media and vice versa. The corresponding mean free time (τ^w) is defined as

$$\tau^w = \frac{l^w}{v_w} = \frac{1}{n\sigma v_w}, \quad (16)$$

where v_w is the incident wave velocity (e.g. Margerin et al. 2000). The mean free time indicates the average time interval between scattering events. Notice that we will use a random variable called free time in the following Monte Carlo simulation (Section 3), and the free time is a time interval between two random scattering events. An important ingredient that differentiates our approach from Maeda et al. (2008) is that we allow the depth-dependent scattering properties for body waves (e.g. σ_ρ^{ShR} and σ_ρ^{Sh}). This depth dependence is related to the coupling of body and Rayleigh waves.

2.5 Theoretical equipartition value

We can calculate the theoretical equipartition energy ratio between two types of multiply-scattered waves. For example, one can calculate the energy ratio between multiply-scattered P and S waves based on the scattering relationship between the two types of body waves (e.g. Weaver 1982). Following the reciprocity relationship in Margerin et al. (2019) and ignoring P-S coupling at the free surface, we write the equipartition energy ratio between multiply-

scattered body and Rayleigh waves as

$$\frac{\bar{\bar{E}}_R}{\bar{E}_P} = \int_0^\infty \frac{\tau_\rho^{RP}(\omega)}{\tau_\rho^{PR}(z_s, \omega)} dz_s = \int_0^\infty \frac{\sigma_\rho^{PR}(z_s, \omega) \alpha_0}{\sigma_\rho^{RP}(\omega) U_R} dz_s = \frac{\pi \alpha_0^3}{\omega c_R U_R}, \quad (17)$$

$$\frac{\bar{\bar{E}}_R}{\bar{E}_{Sv}} = \int_0^\infty \frac{\tau_\rho^{RSv}(\omega)}{\tau_\rho^{SvR}(z_s, \omega)} dz_s = \int_0^\infty \frac{\sigma_\rho^{SvR}(z_s, \omega) \beta_0}{\sigma_\rho^{RSv}(\omega) U_R} dz_s = \frac{\pi \beta_0^3}{\omega c_R U_R}, \quad (18)$$

$$\frac{\bar{\bar{E}}_R}{\bar{E}_{Sh}} = \int_0^\infty \frac{\tau_\rho^{RSh}(\omega)}{\tau_\rho^{ShR}(z_s, \omega)} dz_s = \int_0^\infty \frac{\sigma_\rho^{ShR}(z_s, \omega) \beta_0}{\sigma_\rho^{RSh}(\omega) U_R} dz_s = \frac{\pi \beta_0^3}{\omega c_R U_R}, \quad (19)$$

where $\bar{\bar{E}}_R$ is the total Rayleigh-wave energy over the whole medium, and $\bar{E}_P$ is an integral of P-wave energy over a constant-depth plane and thus is the energy density at the depth. The body-wave energy densities are homogeneous at all depths in the equipartition regime (Margerin et al. 2019), and we validate this in Section 3. U_R is equal to c_R in a homogeneous isotropic elastic medium, but this is not the case in heterogeneous media. The equipartition relationships (Equation 17-19) hold not only for density perturbations, but also for perturbations in the Lamé parameter and shear modulus (Appendix B).

It is not straightforward to combine mode conversion (i.e. P-Sv coupling) at the free surface with the reciprocity relationship when one derives the equipartition ratios (e.g. Shapiro et al. 2000). In order to consider the mode conversion, one needs to adopt another approach also mentioned in Margerin et al. (2019), the density of state (DOS) formulation. We use density of state in the equipartition derivation and achieve the same equipartition ratios (Equations 17-19) in Appendix C. We emphasize that, in a statistically uniform elastic halfspace, the equipartition ratios do not depend on the nature of the disorder.

3 MONTE CARLO SIMULATION

We simulate multiple scattering with a Monte Carlo method. The Monte Carlo simulation method has been applied to multiply scattered acoustic/elastic body waves (e.g. Hoshiya 1991; Margerin et al. 2000). We use this method to simulate multiply-scattered body and Rayleigh waves in a statistically uniform isotropic elastic medium filled with point scatterers. The idea underlying the Monte Carlo simulation is to simulate the propagation and scattering of wave energy as a random walk for a particle and repeat the random walk N times independently (Algorithm 1). After the N simulations, we count how many body and Rayleigh particles exist at each time step and interpret the body and Rayleigh particle numbers as the body- and Rayleigh-wave energy, respectively. Furthermore, by discretizing the 3D medium into a grid and recording changes of the particle numbers at each grid cell with time, we estimate the evolution of wave energy in time and space.

We divide one simulation process into four parts and introduce them separately. Before the simulations start, we need to calculate the cross sections and the mean free times for all possible types of scattering. For perturbations in density or shear modulus, P, Sv, Sh and Rayleigh waves can all be generated during the scattering process; for perturbations in Lamé parameter, only P and Rayleigh waves are generated by the scattering.

3.1 Initialization

We launch a particle at the source location in the beginning of one simulation. The particle can be a body (P/Sv/Sh) or Rayleigh wave (Algorithm 2). We can model different source mechanisms by changing initial wave types (e.g. Margerin et al. 2000) and propagation directions (i.e. azimuth and colatitude). For example, if the source is an explosion, we can set that only P waves are generated at the source location. The P-wave initial azimuths are randomly generated with a uniform probability distribution between 0 and 2π , and the cosines of the P-wave initial colatitudes are randomly generated from a uniform distribution between -1 and 1 (Algorithm 2). For a shear-force source like a fault, all types of waves are randomly selected in proportions equal to their respective radiated energy. Based on the initial wave type, we compute a random free time (T) which indicates the travel time before the next scattering happens. We will cover the details of free time in the next section (Section 3.2). We also calculate the wave propagation vector (k_x, k_y, k_z) based on the propagation azimuths and colatitudes.

3.2 Effective cross section and mean free time

The initialized particle propagates during the random free time T . We compute T as $T = -\tau^w \ln(rand)$ where $rand$ is a random number with a uniform probability distribution from 0 to 1 (e.g. Hoshiaba 1991), and w indicates a body (B) or Rayleigh wave (R). We directly follow the computation for Rayleigh-wave free time but not for the body-wave. Calculation of the body-wave free time between two scattering events is not straightforward, since the body-wave mean free time (τ^B e.g. τ_ρ^{Sh}) varies with depth (Section 2.4). This is because τ_ρ^{Sh} is inversely proportional to σ_ρ^{Sh} , where σ_ρ^{Sh} includes the depth-dependent σ_ρ^{ShR} . Thus, calculation of the body-wave free time requires tracking of the body-wave depth in order to integrate the variation of the mean free time in the propagation. To address this difficulty, we adopt a trick called delta collisions (Lux & Koblinger 1991). The idea of delta collisions is to impose an effective and constant cross section (σ^{Be} where e stands for 'effective') and mean free time. To compensate for the difference between σ^{Be} and the real cross section at a given

Algorithm 1 Monte Carlo simulation algorithm

$\sigma^{Be} = \sum_{B'} \sigma^{BB'} + \max[\sigma^{BR}(z)]$ ▷ Calculating effective body-wave cross section
▷ B and B' can be any possible body wave in scattering, P, Sv or Sh.
 $\tau^{Be} = 1/n/\sigma^{Be}/vb$ ▷ Effective body-wave mean free time
 $\sigma^R = \sigma^{RR} + \sum_B \sigma^{RB}$ ▷ Rayleigh wave cross section
 $\tau^R = 1/n/\sigma^R/vr$ ▷ Rayleigh wave mean free time
 Set dt, the time step for recording particle numbers for each wave mode, P, Sv, Sh and R
for $i = 1 : N$ th simulation **do**
 [mode T azi0 kx ky kz] = Initialization() ▷ Wave mode, free time, propagation azimuth and vector
 Set x, y and z at the source location
 while itime < Nstep **do** ▷ i th simulation starts
 if mode == B **then** ▷ Body-wave propagation
 if $T > \text{deltat}$ **then** ▷ No scattering happen
 $x = x + \text{deltat} * vb * kx$; $y = y + \text{deltat} * vb * ky$; $z = z + \text{deltat} * vb * kz$
 if $z < 0$ **then** ▷ Encounter the free surface
 FreeSurfaceBoundaryCondition
 itime = itime + 1 ▷ Record body-wave type at this time point
 $T = T - \text{deltat}$
 deltat = dt
 else ▷ A scattering will happen
 $x = x + T * vb * kx$; $y = y + T * vb * ky$; $z = z + T * vb * kz$
 if $z < 0$ **then** ▷ Encounter the free surface
 FreeSurfaceBoundaryCondition
 deltat = deltat - T
 [mode T azi0 kx ky kz] = scatterb(azi0) ▷ Body-wave scattering
 if mode == R **then** ▷ Rayleigh-wave propagation
 if $T > \text{deltat}$ **then** ▷ No scattering happen
 $x = x + \text{deltat} * vr * kx$; $y = y + \text{deltat} * vr * ky$
 itime = itime + 1 ▷ Record Rayleigh wave type at this time point
 $T = T - \text{deltat}$
 deltat = dt
 else ▷ A scattering will happen
 $x = x + T * vr * kx$; $y = y + T * vr * ky$
 deltat = deltat - T
 [mode T azi0 kz ky kz z] = scatterr(azi0) ▷ Rayleigh-wave scattering

Algorithm 2 Simulation initialization: $[\text{mode } T \text{ azi0 } kx \text{ ky } kz] = \text{Initialization}()$

 Generate a particle; its **mode** can be a body (B = P/Sv/Sh) or Rayleigh (R) wave

if mode == B **then**
 $T = -\tau^{Be} * \ln(rand)$ ▷ Generate a random free time from a random number
 $ang = \arccos(-1+2*rand)$ ▷ A random colatitude in $[0, \pi]$
 $azi0 = 2*\pi*rand$ ▷ A random propagation azimuth in $[0, 2\pi]$
 $kx = \sin(ang)*\cos(azi0)$ ▷ Body-wave propagation vector in Cartesian coordinates
 $ky = \sin(ang)*\sin(azi0)$
 $kz = \cos(ang)$
else
 $T = -\tau^R * \ln(rand)$
 $azi0 = 2*\pi*rand$ ▷ A random propagation azimuth in $[0, 2\pi]$
 $kx = \cos(azi0)$ ▷ Rayleigh-wave propagation vector in Cartesian coordinates
 $ky = \sin(azi0)$
 $deltat = dt$

depth, we introduce an imaginary scattering part into the body-wave scattering process. The probability that the imaginary scattering event occurs is determined by the difference ($1 - prs$ in Algorithm 3) between σ^{Be} and $\sigma^B(z)$. The imaginary scattering does not change the body-wave propagation direction. Notice that we do not need to introduce the effective mean free time for Rayleigh waves because both $\bar{\sigma}^{RB}$ and $\bar{\sigma}^{RR}$ (e.g. Equation 12) are independent of depth.

3.3 Scattering

After propagating for time T , the particle encounters a scatterer/perturbation, and scattering occurs. We generate a uniformly distributed random value in the range $[0, 1]$ to simulate all possible conversions and determine the scattered wave type (Algorithms 3 and 4). Notice that for incident Rayleigh particles, if a RB conversion happens, we re-inject the scattered body particle at a depth based on the distribution of σ^{RB} as a function of depth (Appendix D). We generate the scattering azimuths and colatitudes (ξ_1 & ψ_1 in Section 2 or azi & ang in the pseudocode) of scattered waves based on the probabilistic interpretation of scattering cross sections (Appendix E). We add the scattering azimuths to the incident azimuth to achieve the propagation azimuth. Due to the isotropic incident angle assumption (Section 2.3), we do not need the incident angles in this part. We discuss this assumption in Section 5.1. Based on

the type of scattered wave, we generate a new value for T to determine the propagation time before the next scattering event.

Algorithm 3 Body-wave scattering subprogram: [mode T azi0 kx ky kz] = scatterb(azi0)

$\sigma^B(z) = \sigma^{BR}(z) + \sum_{B'} \sigma^{BB'}$ $\triangleright$ Cross section for all possible scattering at this depth

$prs = \sigma^B(z)/\sigma^{Be}$ $\triangleright$ Probability that scattering happening

if $rand < prs$ **then**

 Generate a new random number, $rand$ $\triangleright$ determine the scattered mode

if $rand < \sigma^{BP}/\sigma^B(z)$ **then** $\triangleright$ Possibility for BP scattering

 mode = P $\triangleright$ scattered P wave, $B' = P$

if $\sigma^{BP}/\sigma^B(z) < rand < (\sigma^{BP} + \sigma^{BSv})/\sigma^B(z)$ **then** $\triangleright$ Possibility for BSv scattering

 mode = Sv $\triangleright$ scattered Sv wave, $B' = Sv$

if $(\sigma^{BP} + \sigma^{BSv})/\sigma^B(z) < rand < (\sigma^{BP} + \sigma^{BSv} + \sigma^{BSH})/\sigma^B(z)$ **then**

$\triangleright$ Possibility for BSv scattering

 mode = Sh $\triangleright$ scattered Sh wave, $B' = Sh$

$T = -\tau^{B'e} * \ln(rand)$ $\triangleright$ Generate a random free time from a new random number

 Generating azi and ang based on probability distributions (Appendix E)

 azi0 = azi0 + azi

 kx = sin(ang)*cos(azi0) $\triangleright$ Body wave propagation vector in Cartesian coordinates

 ky = sin(ang)*sin(azi0)

 kz = cos(ang)

if $(\sigma^{BP} + \sigma^{BSv} + \sigma^{BSH})/\sigma^B(z) < rand$ **then** $\triangleright$ BR scattering

 mode = R

$T = -\tau^R * \ln(rand)$

 Generate azi based on probability distributions (Appendix E)

 azi0 = azi0 + azi

 kx = cos(azi0) $\triangleright$ Rayleigh-wave propagation vector in Cartesian coordinates

 ky = sin(azi0)

else $\triangleright$ Imaginary scattering happens

 mode = B

$T = -\tau^{Be} * \ln(rand)$ $\triangleright$ The propagation vector and direction stay the same

Algorithm 4 Rayleigh-wave scattering subprogram: $[\text{mode } T \text{ azi0 } kx \text{ ky } kz \text{ z}] = \text{scatterr}(\text{azi0})$

```

zvec = 0 : Dz : zmax          ▷ The depth vector, from 0 to zmax, for injecting body wave
if  $rand < \sigma^{RR}/\sigma^R$  then                                ▷ RR scattering
    mode = R
     $T = -\tau^R * \ln(rand)$                                 ▷ Generate a random free time from a random number
    Generate azi based on probability distributions (Appendix E)
    azi0 = azi0 + azi
     $kx = \cos(azi0)$                                 ▷ Rayleigh-wave propagation vector in Cartesian coordinates
     $ky = \sin(azi0)$ 
else                                ▷ RB scattering
    if  $rand < (\sigma^{RR} + \sigma^{RP})/\sigma^R$  then
        mode = P                                ▷ RP scattering,  $B = P$ 
    if  $(\sigma^{RR} + \sigma^{RP})/\sigma^R < rand < (\sigma^{RR} + \sigma^{RP} + \sigma^{RSv})/\sigma^R$  then
        mode = Sv                                ▷ RSv scattering,  $B = Sv$ 
    if  $(\sigma^{RR} + \sigma^{RP} + \sigma^{RSv})/\sigma^R < rand$  then
        mode = Sh                                ▷ RSv scattering,  $B = Sh$ 
     $z = \text{interp1}(\sigma^{RB}(\text{zvec})/\int \sigma^{RB}(z)dz, \text{zvec}, rand)$ 
        ▷ Inject body wave at depth based on RB cross section in depth (Appendix D)
     $T = -\tau^{Be} * \ln(rand)$ 
    Generating azi and ang based on probability distributions (Appendix E)
    azi0 = azi0 + azi
     $kx = \sin(ang)*\cos(azi0)$                                 ▷ Body-wave propagation vectors in Cartesian coordinates
     $ky = \sin(ang)*\sin(azi0)$ 
     $kz = \cos(ang);$ 

```

3.4 Boundary conditions

We assume the free surface is flat and adopt two types of free-surface boundary conditions (FSBCs) in the simulation: mirror-like reflection and mode conversion. The mirror FSBC conserves the wave energy and propagation vector except for the sign of the vertical component. This FSBC does not modify the incident wave type (i.e. no mode conversion). The mode-conversion FSBC allows the wave mode conversion (i.e. P to Sv or Sv to P) based on energy reflection coefficients. Depending on the incident-wave angle and wave type ($B=P/Sv$), we can calculate the corresponding reflection coefficient (R_{BB}) for a reflected wave remaining as the same wave type (e.g. Aki & Richards 2002, Chapter 5.2.2). R_{BB} is the reflected wave

amplitude ratio relative to the incident-wave amplitude. Given the incident-wave intensity is 1, we recognize that the square of the coefficient (R_{BB}^2) is the intensity of the reflection wave and the probability of this reflection. We then generate a random number from a uniform distribution between 0 and 1. If the random number is less than or equal to R_{BB}^2 , no mode conversion happens; otherwise, the incident P or Sv wave will convert to a Sv or P wave, respectively. If the mode conversion happens, we also recalculate the free time for the reflected waves. For the boundary condition in the depth, we assume that body waves can propagate to infinite depth in the simulations.

4 SIMULATION RESULTS

We set the frequency be 1 Hz and choose the medium parameters as follows: $\alpha_0=5$ km/s, $\beta_0=3$ km/s and thus $c_R=2.74$ km/s. We set the medium to be 10 km (zmax in Algorithm 4) thick. We assume that there is no intrinsic attenuation in the medium, which means that the seismic-wave energy will not irreversibly convert to other types of energies. We also assume that the scatterers ($\delta\rho$) are randomly distributed in the medium, and set the perturbation density relative to the background ($\delta\rho/\rho_0$) to 0.2 and a scatterer volume (V) to be 0.5 m^3 . We also set the volume density of scatterers (n) equal to 1 m^{-3} . We compute the Rayleigh-wave eigenfunctions based on these velocities (Appendix A) and calculate all the cross sections and mean free times (Appendix B and Equation 16). The Rayleigh-wave mean free path (l^R) is 35.8 km (Equation 15) and is of the same order of mean free path as in Earth's crust (e.g. Margerin et al. 1999). Note that the ratio between l^R and the Rayleigh-wave wavelength (2.74 km) is 13 and fulfills the condition of application of radiative transfer theory that the mean free path should be much larger than the corresponding wavelengths (e.g. Ryzhik et al. 1996). In the simulation, we place a source at 1 km depth. The source emits P and Rayleigh waves/particles. During the random walk for one particle, we record the location and mode for the particle every 1 s (dt in Algorithm 1). The random walk lasts 3000 s (Nstep=3000 in Algorithm 1). We repeat the random walk 100 million ($N = 10^8$) times. For each wave mode, we count the particles in a certain space (e.g. the shallowest 1km depth of the medium) in all the random walks and then divide the particle number with N to get the wave energy.

We first simulate multiple scattering with the mirror FSBC. At each time step in the simulation, we estimate the body wave energy density as a function of depth ($\overline{E}_B$: $\overline{E}_P$, $\overline{E}_{Sv}$ and $\overline{E}_{Sh}$) by counting the number of body waves per 1 km depth in the medium. We observe that $\overline{E}_B$ at each depth gradually becomes uniform in depth as the simulation time increases (Figure 2). The homogenization of body-wave energy is due to the balance between the RB and

Figure 2. The simulated body-wave energy densities as a function of depth. We plot the energy densities at different simulation time in the unit of Rayleigh-wave mean free time (τ^R): 20, 50, 100 and 200 τ^R . The black curves are from the simulation with the mirror free surface boundary condition (FSBC); the red curves are from the mode-conversion FSBC. We smooth each curve by convolution with a Gaussian filter with a width of one third the Rayleigh-wave wavelength.

BR scattering (Margerin et al. 2019). We calculate the Rayleigh-wave energy ($\bar{E}_R$) by counting the number of Rayleigh waves in the whole medium. We observe that the energy ratios between $\bar{E}_R$ and $\bar{E}_{Sv/h}$ become homogeneous after 50 τ^R , and the energy ratios between $\bar{E}_R$ ($\bar{E}_{Sv/h}$) and $\bar{E}_P$ become constant after 100 τ^R (Figure 3). We determine that the simulation reaches equipartition after all these energy ratios stabilize. All of the stable ratios are close to the corresponding theoretical values with a 4.7% maximum misfit (Table 1).

We switch the FSBC to the mode-conversion case and repeat the simulation. In this simulation, similar to the last one, we observe homogeneous body-wave energies in depth in the equipartition stage (Figure 2). This mode-conversion FSBC provides similar energy partition ratios among Rayleigh and body waves compared to the mirror FSBC simulation (Figure 4 and Table 1). This similarity is not surprising because Trégourès & van Tiggelen (2002) theoretically demonstrated that the mode-conversion (i.e traction free) FSBC does not affect the body-wave energy partition ratios. Here we numerically demonstrate that no matter which FSBC is used, the simulation reaches equipartition. In addition, the body-wave angular distributions on the free surface match Lambert’s cosine law from the diffusion theory (Appendix F).

Figure 3. Temporal evolution of the energy partitioning ratios among Rayleigh, P, and Sv/h waves in the simulation with the mirror FSBC. We estimate $\bar{E}_B$ in the shallowest 1 km depth of the medium. We calculate the simulated energy ratio from the last 50 τ^R simulation results. The theoretical energy ratios are from Equations 17, 18 and 19. We plot the ratios from the simulation results and the equipartition theory in solid and dashed lines, respectively.

5 DISCUSSION

5.1 Body-wave incident angles

We average the incident-angle-dependent cross sections by assuming that the incident body waves are isotropic, i.e. evenly distributed on a unit sphere. We examine this assumption here using our simulation results. We discuss the scattering colatitudes (ψ_1 in Figure 1) because we actually use the colatitudes in simulation of the wave propagation (e.g. $\cos(\psi_1)$). If the scattered-body-wave colatitudes are isotropic, $\cos(\psi_1)$ will be equal to 1 for all incident angles and the incident angles will also be isotropic. The positive and negative cosine values represent down-going and up-going wave propagation, respectively. We divide the potential range for $\cos(\psi_1)$, from -1 to 1, into 180 even bins. At each time step in the simulation, we count the particle (i.e. wave) numbers for all types of body waves in each bin from the free surface to 10 km depth; we then calculate ratios between the particle numbers and the mean of the P particle numbers in all the bins. We finally average the ratios in a time

Figure 4. Temporal evolution of the energy partitioning ratios among Rayleigh, P and Sv/h waves in the simulation with the mode-conversion FSBC. All data processing and figure settings match those in Figures 3.

range when the energy partitioning ratios are stable, such as the last 50 Rayleigh-wave mean free times ($50 \tau^R$). We refer to these averaged ratios with respect to $\cos(\psi_1)$ as angular distributions for each type of wave (Figure 5). Based on the isotropic angular distributions, we expect the P- and Sv-/Sh-wave ratios to be 1 and $(\alpha_0/\beta_0)^3$, respectively. In the two FSBC simulation results, we observe similar angular distributions (Figure 5). The P-wave

Table 1. Misfits in the simulation results. We calculate the absolute difference between the simulated and theoretical energy equipartition values (Figure 3, 4 and 6), and the misfit value is the ratio of the absolute difference relative to the theoretical energy equipartition value. Simulations with the mirror and mode-conversion FSBCs are presented in Section 4. The simulation with isotropic RB scattering is presented in Section 5.1.

Simulation	RP	RSv	RSh	PSv	PSh
Mirror FSBC	4.7%	0	2.2%	4.6%	2.3%
Mode-conversion FSBC	4.6%	0.2%	2.2%	4.6%	2.3%
Isotropic RB	1.1%	0.3%	0.3%	0.9%	0.9%

distributions are almost isotropic with about 10% off than the expectation, 1, near $\cos(\psi_1) = 0$ (i.e. parallel to the free surface, the insets in Figure 5a and b). The Sv-wave ratios are slightly elevated from $\cos(\psi_1) = -1$ to $\cos(\psi_1) = 0$ (i.e. up-going waves); for the down-going waves, the Sv-wave ratios are perturbed from the expected values with 10% as a maximum near $\cos(\psi_1) = 0.05$. The Sh-wave distributions are almost isotropic for all the cosine values and match the theoretical value, $(\alpha_0/\beta_0)^3$.

To investigate reasons for the biases in the angular distributions, we propose two tests. First, we check the body-wave angular distributions when we only have body-wave scattering in the simulation. To do that, we turn off the coupling between body and Rayleigh waves, i.e. no RB or BR scattering. We then run this modified simulation with the mode-conversion FSBC and calculate the angular distributions as above. We observe that all the body-wave angular distributions are isotropic after the simulation reaches equipartition (Figure 5c). This observation fits the generalized diffusion theory for the mode-conversion FSBC (e.g. Trégourès & van Tiggelen 2002) and indicates that the biases are not related to body-wave multiple scattering. Second, we turn on the Rayleigh-wave coupling and require the RP and RSv scattering colatitudes to be isotropic while the RSh scattering is already isotropic from the physics (Figure 5d). We observe that this new simulation also generates isotropic distributions for all body waves. Furthermore, this new simulation provides more accurate energy equipartition ratios than the two in Section 4 (Figure 6 and Table 1). Thus, we conclude that the biases in the body-wave angular distributions in the simulation algorithm are due to the anisotropic RP and RSv scattering colatitude patterns. The isotropic scattering patterns can be used in the multiple scattering simulations as done before (e.g. Sato & Nishino 2002). However, the anisotropic RP and RSv scattering patterns are from the physics and change with depth (Figure E1). Therefore this observation and these biases need to be further investigated and more fully understood. This is a new observation that has not been noted in the literature before.

5.2 Potential improvements on the simulation

The Monte Carlo simulation algorithm presented here can model body/Rayleigh-wave energy propagating and scattering with a flat free surface, but we cannot model other seismic wave phenomena, such as inhomogeneous waves or nongeometric waves. Inhomogeneous waves are due to shallow seismic sources or seismic wave reflections (e.g. Aki & Richards 2002). Inhomogeneous wave reflection at the free surface can generate nongeometric waves (e.g. Hron & Mikhailenko 1981; Roth & Holliger 2000). We can model these wave phenomena using wave

Figure 5. The body-wave angular distributions from the simulation with the mirror FSBC (a), the mode-conversion FSBC (b), the mode-conversion FSBC and no RB or BR scattering (c), and the mode-conversion FSBC and isotropic RB scattering (d). We use anisotropic RB scattering in (a) and (b). The theoretical values for the P and Sh/Sv wave are always 1 and $(\alpha/\beta)^3$ for all $\cos(\psi_1)$, respectively. We plot the distributions from the simulation results and the diffusive theory in solid and dashed lines, respectively. The insets in (a) and (b) show zooms of the P-wave distributions at $\cos(\psi_1) = 0$.

equations, but we have not incorporated these wave phenomena into the radiative transfer theory or Monte Carlo simulations yet. We do not consider complex subsurface media such as lateral heterogeneities (e.g. Yu et al. 2021), interfaces (e.g. Margerin et al. 1998; Sanborn et al. 2017), a topographic free surface (e.g. Snieder 1986b; Takemura et al. 2015; Wang et al. 2015) or intrinsic attenuation (e.g. Zhang et al. 2021) into our simulations yet. Incorporating those into our algorithm is a promising direction for future studies and thus help studies like surface waves in microseisms (e.g. Ziane & Hadziioannou 2019; Gualtieri et al. 2020)

We model Sv and Sh waves separately in our algorithm. However, in practice, S waves are

Figure 6. Temporal evolution of the energy partitioning ratios among Rayleigh, P and Sv/h waves in the simulation with the mode-conversion FSBC and isotropic RB scattering. All data processing and figure settings match those in Figure 3.

commonly combinations of both. One can use the Stokes vector to model the combinations in elastic media (e.g. Turner & Weaver 1995; Margerin et al. 2000). In using that approach, one needs to track not only the body-wave propagation direction as in our algorithm, but also polarization directions. Research regarding incorporation of Rayleigh waves into the Stokes vector is still absent and will be helpful for modelling Rayleigh- and Love-wave multiple scattering due to different polarization S waves.

6 CONCLUSION

We develop a Monte Carlo simulation algorithm to model body- and surface-wave multiple scattering in elastic media. We consider all the possible scattering combinations among P, Sv, Sh and Rayleigh waves, and derive the corresponding cross sections due to perturbations in elastic properties (i.e. density, Lamé parameter and shear modulus). We use these cross sections in the simulation and thus physically incorporate the interaction between body and Rayleigh waves during scattering. The algorithm provides the spatio-temporal evolution of body- and Rayleigh-wave energies. We focus on density perturbations as scatterers and vali-

date the algorithm by comparing the simulation results to the theoretical energy ratios. We numerically demonstrate that the simulations with the mirror and mode-conversion free surface boundary conditions provide similar energy equipartition ratios close to the theoretical equipartition values. In the equipartition state, the body-wave angular distributions on the free surface match Lambert’s cosine law under the two different free surface boundary conditions. Our results also indicate that biases in the simulation results are due to the anisotropic BR scattering angle patterns. Our research provides a new tool to study the multiple scattering phenomena in elastic media, and thus may aid coda wave studies such as Q estimation or interpretation of coda-wave monitoring results.

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8 DATA AVAILABILITY

The data underlying this article are available in the article.

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APPENDIX A: RAYLEIGH WAVE EIGENFUNCTIONS

Rayleigh waves possess displacements in the vertical (Z) and radial (R) directions. In a 1D elastic medium, one can write the two component displacement at frequency ω and depth z as

$$u_R = r_1(z, \omega) \exp[i(k_R \Delta - \omega t)], \quad (\text{A.1})$$

$$u_Z = r_2(z, \omega) \exp[i(k_R \Delta - \omega t)], \quad (\text{A.2})$$

where r_1 and r_2 are the eigenfunctions, k_R is the Rayleigh-wave wavenumber, and Δ is the propagation distance (Aki & Richards 2002, Chapter 7.2). One calculates the two eigenfunctions based on boundary conditions: vanishing traction at the free surface and zero displacement at infinity (e.g. Aki & Richards 2002, Chapter 7.2.1). In a homogeneous halfspace, the

analytical expressions for the eigenfunctions are

$$r_1(z, \omega) = -k_R \exp(-k_R \sqrt{1 - \frac{c_R^2}{\alpha_0^2}} z) + k_R \frac{2\beta_0^2 - c_R^2}{2\beta_0^2} \exp(-k_R \sqrt{1 - \frac{c_R^2}{\beta_0^2}} z), \quad (\text{A.3})$$

and

$$r_2(z, \omega) = -k_R \sqrt{1 - \frac{c_R^2}{\alpha_0^2}} \exp(-k_R \sqrt{1 - \frac{c_R^2}{\alpha_0^2}} z) + k_R \frac{2\sqrt{1 - \frac{c_R^2}{\alpha_0^2}}}{2 - \frac{c_R^2}{\beta_0^2}} \exp(-k_R \sqrt{1 - \frac{c_R^2}{\beta_0^2}} z). \quad (\text{A.4})$$

We calculate the eigenfunctions for the velocity model where $\alpha_0=5$ km/s and $\beta_0=3$ km/s (Figure A1), and we use the eigenfunctions in the scattering amplitudes (e.g. Equation 7) and cross sections (e.g. Equation 10).

APPENDIX B: SCATTERING CROSS SECTIONS

B1 Body-to-Rayleigh-wave cross sections

For scattering due to perturbations in the Lamé parameter (i.e. $\delta\lambda$),

$$\sigma_\lambda^{PR} = \frac{k_P^3(\alpha_0^2 - 2\beta_0^2)^2}{4c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left(r_1 + \frac{1}{k_R} \frac{\partial r_2}{\partial z} \right)^2 V^2 \left(\frac{\delta\lambda}{\lambda_0} \right)^2, \quad (\text{B.1})$$

$$\sigma_\lambda^{SvR} = \sigma_\lambda^{ShR} = 0. \quad (\text{B.2})$$

For $\delta\rho$ scatters,

$$\sigma_\rho^{PR} = \frac{\omega^3}{8\alpha_0 c_R U_R \int (r_1^2 + r_2^2) dz} [r_1^2 \sin^2(\psi_0) + 2r_2^2 \cos^2(\psi_0)] V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.3})$$

$$\sigma_\rho^{SvR} = \frac{\omega^3}{8\beta_0 c_R U_R \int (r_1^2 + r_2^2) dz} [r_1^2 \cos^2(\psi_0) + 2r_2^2 \sin^2(\psi_0)] V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.4})$$

$$\sigma_\rho^{ShR} = \frac{\omega^3}{8\beta_0 c_R U_R \int (r_1^2 + r_2^2) dz} r_1^2 V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.5})$$

where ψ_0 is the body-wave incident angle (Figure 1). After averaging over incident angles,

$$\tilde{\sigma}_\rho^{PR} = \frac{1}{\int_0^\pi \sin(\psi_0) d\psi_0} \int_0^\pi \sigma_\rho^{PR} \sin(\psi_0) d\psi_0 = \frac{\omega^3}{12\alpha_0 c_R U_R \int (r_1^2 + r_2^2) dz} (r_1^2 + r_2^2) V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.6})$$

$$\tilde{\sigma}_\rho^{SvR} = \frac{1}{\int_0^\pi \sin(\psi_0) d\psi_0} \int_0^\pi \sigma_\rho^{SvR} \sin(\psi_0) d\psi_0 = \frac{\omega^3}{24\beta_0 c_R U_R \int (r_1^2 + r_2^2) dz} (r_1^2 + 4r_2^2) V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.7})$$

$$\tilde{\sigma}_\rho^{ShR} = \sigma_\rho^{ShR}. \quad (\text{B.8})$$

Figure A1. Radial (r_1) and vertical (r_2) eigenfunctions vary with depth at 1 Hz. The eigenfunction values are normalized by the absolute value of r_1 at the free surface ($z = 0$). The depth axes are Rayleigh-wave wavelength (λ_R) and kilometers to demonstrate how shallow scatterers must be in order to generate Rayleigh waves.

647

For perturbations in shear modulus ($\delta\mu$),

$$\sigma_\mu^{PR} = \frac{\omega^3 \beta_0^4}{8\alpha_0^3 c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left[3r_1^2 \sin^4(\psi_0) + \frac{8}{k_R^2} \left(\frac{\partial r_2}{\partial z} \right)^2 \cos^4(\psi_0) + \frac{8r_1}{k_R} \frac{\partial r_2}{\partial z} \sin^2(\psi_0) \cos^2(\psi_0) \right. \\ \left. + \frac{1}{k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 \sin^2(2\psi_0) + r_2^2 \sin^2(2\psi_0) - \frac{2}{k_R} \frac{\partial r_1}{\partial z} r_2 \sin^2(2\psi_0) \right] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.9})$$

$$\sigma_\mu^{SvR} = \frac{\omega^3 \beta_0}{8c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left[\frac{3}{4} r_1^2 \sin^2(2\psi_0) + \frac{2}{k_R^2} \left(\frac{\partial r_2}{\partial z} \right)^2 \sin^2(2\psi_0) - \frac{2}{k_R} r_1 \frac{\partial r_2}{\partial z} \sin^2(2\psi_0) \right. \\ \left. + r_2^2 \cos^2(2\psi_0) + \frac{1}{k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 \cos^2(2\psi_0) - \frac{2}{k_R} \frac{\partial r_1}{\partial z} r_2 \cos^2(2\psi_0) \right] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.10})$$

$$\sigma_\mu^{ShR} = \frac{\omega^3 \beta_0}{8c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left[r_1^2 \sin^2(\psi_0) + r_2^2 \cos^2(\psi_0) + \frac{1}{k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 - \frac{2}{k_R} \frac{\partial r_1}{\partial z} r_2 \cos(\psi_0) \right] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2. \quad (\text{B.11})$$

648 After averaging over incident angles,

$$\tilde{\sigma}_\mu^{PR} = \frac{\omega^3 \beta_0^4}{15\alpha_0^3 c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left[3r_1^2 + \frac{3}{k_R^2} \left(\frac{\partial r_2}{\partial z} \right)^2 + \frac{2r_1}{k_R} \frac{\partial r_2}{\partial z} + \frac{1}{k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 + r_2^2 - \frac{2}{k_R} \frac{\partial r_1}{\partial z} r_2 \right] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.12})$$

$$\tilde{\sigma}_\mu^{SvR} = \frac{\omega^3 \beta_0}{c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left[\frac{r_1^2}{20} + \frac{2}{15k_R^2} \left(\frac{\partial r_2}{\partial z} \right)^2 - \frac{2}{15k_R} r_1 \frac{\partial r_2}{\partial z} + \frac{7}{120} r_2^2 + \frac{7}{120k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 - \frac{7}{60k_R} \frac{\partial r_1}{\partial z} r_2 \right] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.13})$$

$$\tilde{\sigma}_\mu^{ShR} = \frac{\omega^3 \beta_0}{16c_R U_R^3 \int (r_1^2 + r_2^2) dz} \left[\frac{4}{3} r_1^2 + \frac{2}{3} r_2^2 + \frac{2}{k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 \right] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2. \quad (\text{B.14})$$

649 B2 Rayleigh-to-body-wave cross sections

650 For perturbations in the Lamé parameter ($\delta\lambda$),

$$\bar{\sigma}_\lambda^{RP} = \frac{k_P^4 (\alpha_0^2 - 2\beta_0^2)^2}{4\pi\alpha_0 c_R^2 U_R \int (r_1^2 + r_2^2) dz} \int \left(r_1 + \frac{1}{k_R} \frac{\partial r_2}{\partial z} \right)^2 dz_s V^2 \left(\frac{\delta\lambda}{\lambda_0} \right)^2, \quad (\text{B.15})$$

$$\sigma_\lambda^{RSv} = \sigma_\lambda^{RSh} = 0, \quad (\text{B.16})$$

651 where $\bar{\sigma}$ is the integral of σ over depth (e.g. Equation 12).

652 For perturbations in density ($\delta\rho$),

$$\bar{\sigma}_\rho^{RP} = \frac{\omega k_P^3}{12\pi U_R} V^2 \left(\frac{\delta\rho}{\delta\rho_0} \right)^2, \quad (\text{B.17})$$

$$\bar{\sigma}_\rho^{RSv} = \frac{\omega k_S^3}{24\pi U_R} \frac{\int (r_1^2 + 4r_2^2) dz_s}{\int (r_1^2 + r_2^2) dz} V^2 \left(\frac{\delta\rho}{\delta\rho_0} \right)^2, \quad (\text{B.18})$$

$$\bar{\sigma}_\rho^{RSh} = \frac{\omega k_S^3}{8\pi U_R} \frac{\int r_1^2 dz_s}{\int (r_1^2 + r_2^2) dz} V^2 \left(\frac{\delta\rho}{\delta\rho_0} \right)^2. \quad (\text{B.19})$$

653 For perturbations in shear modulus ($\delta\mu$),

$$\bar{\sigma}_\mu^{RP} = \frac{k_P^4 \beta_0^4}{15\pi\alpha_0 c_R^2 U_R \int (r_1^2 + r_2^2) dz} \int \left[3r_1^2 + \frac{3}{k_R^2} \left(\frac{\partial r_2}{\partial z} \right)^2 + 2\frac{r_1}{k_R} \frac{\partial r_2}{\partial z} + \frac{1}{k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 + r_2^2 - \frac{2}{k_R} \frac{\partial r_1}{\partial z} r_2 \right] dz_s V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.20})$$

$$\bar{\sigma}_\mu^{RSv} = \frac{\omega^3 k_S}{\pi c_R^2 U_R \int (r_1^2 + r_2^2) dz} \int \left[\frac{1}{20} r_1^2 + \frac{2}{15k_R^2} \left(\frac{\partial r_2}{\partial z} \right)^2 - \frac{2}{15k_R} r_1 \frac{\partial r_2}{\partial z} + \frac{7}{120} r_2^2 + \frac{7}{120k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 - \frac{7}{60k_R} \frac{\partial r_1}{\partial z} r_2 \right] dz_s V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.21})$$

$$\bar{\sigma}_\mu^{RSh} = \frac{\omega^3 k_S}{\pi c_R^2 U_R \int (r_1^2 + r_2^2) dz} \int \left[\frac{r_1^2}{12} + \frac{r_2^2}{24} + \frac{1}{8k_R^2} \left(\frac{\partial r_1}{\partial z} \right)^2 \right] dz_s V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2. \quad (\text{B.22})$$

B3 Rayleigh-to-Rayleigh-wave cross sections

$$\bar{\sigma}_{\lambda}^{RR} = \frac{\omega^3(\alpha_0^2 - 2\beta_0^2)^2}{4c_R^5 U_R^2 [\int (r_1^2 + r_2^2) dz]^2} \int \left(r_1 + \frac{1}{k_R} \frac{\partial r_2}{\partial z} \right)^4 dz_s V^2 \left(\frac{\delta \lambda}{\lambda_0} \right)^2, \quad (\text{B.23})$$

$$\bar{\sigma}_{\rho}^{RR} = \frac{\omega^3}{8c_R U_R^2 [\int (r_1^2 + r_2^2) dz]^2} \int (r_1^4 + 2r_2^4) dz_s V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.24})$$

$$\bar{\sigma}_{\mu}^{RR} = \frac{\omega^3 \beta_0^4}{8c_R U_R^2 [\int (r_1^2 + r_2^2) dz]^2} \int \left[3r_1^4 + \left(r_2 - \frac{1}{k_R} \frac{\partial r_1}{\partial z} \right)^4 + \frac{8}{k_R^4} \left(\frac{\partial r_2}{\partial z} \right)^4 + \frac{8}{k_R^2} r_1^2 \left(\frac{\partial r_2}{\partial z} \right)^2 \right] dz_s V^2 \left(\frac{\delta \mu}{\mu_0} \right)^2. \quad (\text{B.25})$$

B4 Body-to-body-wave cross sections

For perturbations in the Lamé parameter ($\delta \lambda$),

$$\sigma_{\lambda}^{PP} = \frac{k_P^4}{4\pi} \left(\frac{\alpha_0^2 - 2\beta_0^2}{\alpha_0^2} \right)^2 V^2 \left(\frac{\delta \lambda}{\lambda_0} \right)^2, \quad (\text{B.26})$$

$$\sigma_{\lambda}^{PSh} = \sigma_{\lambda}^{PSv} = \sigma_{\lambda}^{ShP} = \sigma_{\lambda}^{SvP} = 0. \quad (\text{B.27})$$

For perturbations in the density ($\delta \rho$), we write the cross sections

$$\sigma_{\rho}^{PP} = \frac{k_P^4}{12\pi} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.28})$$

$$\sigma_{\rho}^{PSv} = \frac{\beta_0 k_s^4}{24\pi \alpha_0} [1 + 3 \cos^2(\psi_0)] V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.29})$$

$$\sigma_{\rho}^{PSh} = \frac{\beta_0 k_s^4}{8\pi \alpha_0} \sin^2(\psi_0) V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.30})$$

$$\sigma_{\rho}^{SvP} = \sigma_{\rho}^{ShP} = \frac{\alpha_0 k_P^4}{12\pi \beta_0} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.31})$$

$$\sigma_{\rho}^{SvSv} = \frac{k_S^4}{24\pi} [1 + 3 \sin^2(\psi_0)] V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.32})$$

$$\sigma_{\rho}^{SvSh} = \frac{k_S^4}{8\pi} \cos^2(\psi_0) V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.33})$$

$$\sigma_{\rho}^{ShSv} = \frac{k_S^4}{24\pi} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2, \quad (\text{B.34})$$

$$\sigma_{\rho}^{ShSh} = \frac{k_S^4}{8\pi} V^2 \left(\frac{\delta \rho}{\rho_0} \right)^2. \quad (\text{B.35})$$

658 and the averaged cross sections over incident angles

$$\tilde{\sigma}_\rho^{PSv} = \frac{\beta_0 k_s^4}{12\pi\alpha_0} V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.36})$$

$$\tilde{\sigma}_\rho^{PSh} = \frac{\beta_0 k_s^4}{12\pi\alpha_0} V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.37})$$

$$\tilde{\sigma}_\rho^{SvSv} = \frac{k_S^4}{8\pi} V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.38})$$

$$\tilde{\sigma}_\rho^{SvSh} = \frac{k_S^4}{24\pi} V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2. \quad (\text{B.39})$$

659 For perturbations in shear modulus ($\delta\mu$),

$$\sigma_\mu^{PP} = \frac{k_P^4 \beta_0^4}{5\pi\alpha_0^4} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.40})$$

$$\sigma_\mu^{PSv} = \frac{\beta_0 k_S^2 k_P^2}{60\pi\alpha_0} [3 + 5 \cos^4(\psi_0)] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.41})$$

$$\sigma_\mu^{PSh} = \frac{\beta_0 k_S^2 k_P^2}{12\pi\alpha_0} [\sin^4(\psi_0) + 2 \sin^2(\psi_0) \cos^2(\psi_0)] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.42})$$

$$\sigma_\mu^{SvP} = \sigma_\mu^{ShP} = \frac{1}{15} \frac{k_P^4 \beta_0}{\pi\alpha_0} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.43})$$

$$\sigma_\mu^{SvSv} = \frac{k_S^4}{120\pi} [38 \sin^2(\psi_0) \cos^2(\psi_0) + 7 \cos^2(2\psi_0)] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.44})$$

$$\sigma_\mu^{SvSh} = \frac{k_S^4}{48\pi} [1 + \cos^2(2\psi_0)] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.45})$$

$$\sigma_\mu^{ShSv} = \frac{k_S^4}{120\pi} [2 + 5 \cos^2(\psi_0)] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.46})$$

$$\sigma_\mu^{ShSh} = \frac{k_S^4}{24\pi} [1 + \sin^2(\psi_0)] V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.47})$$

660 and

$$\tilde{\sigma}_\mu^{PSv} = \frac{\beta_0 k_S^2 k_P^2}{15\pi\alpha_0} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.48})$$

$$\tilde{\sigma}_\mu^{PSh} = \frac{\beta_0 k_S^2 k_P^2}{15\pi\alpha_0} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.49})$$

$$\tilde{\sigma}_\mu^{SvSv} = \frac{5k_S^4}{72\pi} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.50})$$

$$\tilde{\sigma}_\mu^{SvSh} = \frac{11k_S^4}{360\pi} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.51})$$

$$\tilde{\sigma}_\mu^{ShSv} = \frac{11k_S^4}{360\pi} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2, \quad (\text{B.52})$$

$$\tilde{\sigma}_\mu^{ShSh} = \frac{5k_S^4}{72\pi} V^2 \left(\frac{\delta\mu}{\mu_0} \right)^2. \quad (\text{B.53})$$

B5 Validation

We observe that

$$\frac{\sigma_{\rho}^{PSv} + \sigma_{\rho}^{PSh}}{\sigma_{\rho}^{SvP}} = \frac{\sigma_{\mu}^{PSv} + \sigma_{\mu}^{PSh}}{\sigma_{\mu}^{SvP}} = 2 \left(\frac{\alpha_0}{\beta_0} \right)^2. \quad (\text{B.54})$$

The above relationship agrees with previous research about the cross-section ratios between P and S waves (Aki 1992). We can further write

$$\sigma_{\rho}^{SS} = \sigma_{\rho}^{SvSv} + \sigma_{\rho}^{SvSh} = \sigma_{\rho}^{ShSv} + \sigma_{\rho}^{ShSh} = \frac{k_S^4}{6\pi} V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2, \quad (\text{B.55})$$

$$\sigma_{\mu}^{SS} = \sigma_{\mu}^{SvSv} + \sigma_{\mu}^{SvSh} = \sigma_{\mu}^{ShSv} + \sigma_{\mu}^{ShSh} = \frac{k_S^4}{10\pi} V^2 \left(\frac{\delta\rho}{\rho_0} \right)^2. \quad (\text{B.56})$$

We observe that the two body-wave expressions above, along with the expressions of $\sigma^{PP}, \sigma^{SvP}, \sigma^{ShP}$ and $\sigma^{PSv} + \sigma^{PSh}$ due to $\delta\lambda/\delta\rho/\delta\mu$ are the same as the body-wave cross-section formulas in Margerin et al. (2000). Notice that the cross sections here are not averaged along incident angles.

APPENDIX C: EQUIPARTITION FROM THE DENSITY OF STATE

A basic principle in multiple scattering theory is equipartition. It stipulates that the correlation function of a diffuse field is proportional to the imaginary part of the Green's function of the underlying wave equation. The trace of the imaginary part of the local Green's function is proportional to the (local) density of states (DOS) that counts all possible modes of propagation. Hence, the energy partitioning among different propagation modes in the diffuse regime can be obtained from the DOS. Formally, the DOS can be written as

$$\text{DOS} = -\frac{2\omega}{\pi} \text{Tr} \text{Im} G(\mathbf{x}, \mathbf{x}; \omega) = 2\omega \sum_n \delta(\omega^2 - \lambda_n) |\phi_n(\mathbf{x})|^2 \quad (\text{C.1})$$

for positive angular frequency ω . In the last equality, the index n runs over all possible eigenmodes of the elastodynamic operator $L = -\alpha^2 \nabla \nabla \cdot + \beta^2 \nabla \times \nabla \times$ with eigenvalues λ_n and displacement eigenfunction ϕ_n . Notice that using λ to represent eigenvalues is custom in the DOS theory and we only use this representation in this appendix. These eigenfunctions must be normalized in the sense of the scalar product $\langle \phi_n | \phi'_n \rangle = \int d^3r \phi_n(\mathbf{x}) \phi'_n(\mathbf{x})^* = \delta_{n,n'}$. In our application, the index n will be continuous and all discrete sums become integrals as shown below. The eigenfunctions of the operator L in an elastic halfspace bounded by a free surface are plane Rayleigh wave and body-wave modes composed of an incident (normalized) plane wave of a given polarization (P/Sv/Sh) together with its reflections. A rigorous diagonalization of the operator L in a halfspace bounded by a free surface can be found in Sécher (1998) and

more details about the eigenvalues and eigenfunctions can be found in Margerin (2009). We will examine the contributions of the different types of waves to the DOS using a classical seismological approach in this section.

We first compute the DOS per unit surface for Rayleigh waves by integrating Equation C.1 over depth. Taking into account that a Rayleigh-wave eigenmode with horizontal wavevector (k_x, k_y) is associated to the eigenvalue $\lambda = c_r^2(k_x^2 + k_y^2)$ and the normalization condition, we find:

$$N_R = 2\omega \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{\delta(\omega^2 - c_r^2(k_x^2 + k_y^2))}{(2\pi)^2}, \quad (C.2)$$

$$= \frac{\omega}{2\pi c_R^2}.$$

In the first line of Equation C.2, the factor $(2\pi)^{-2}$ inside the integral is inherited from the normalization condition for plane waves in 2-D. Note that N_R is a DOS per unit surface per unit frequency.

Let us now examine the case for Sh waves. From the basic analysis of free-surface reflection, we know that an Sh eigenfunction is of the form:

$$\phi_{Sh}(\mathbf{x}) = \frac{(e^{-iqz} + e^{iqz})e^{i(k_x x + k_y y)}}{(2\pi)^{3/2}} \mathbf{e}^{Sh}, \quad (C.3)$$

which corresponds to the sum of an incident and a reflected plane wave with horizontal unit polarization vector $\mathbf{e}^{Sh}$ in the direction $(k_y, -k_x, 0)$. We take the vertical axis oriented positively downward, so that a wavenumber $-q < 0$ (i.e. positive q) represents a up-going wave. The eigenvalue associated to ϕ_{Sh} is $\lambda = \beta_0^2(k_x^2 + k_y^2 + q^2)$ and the prefactor $(2\pi)^{-3/2}$ guarantees that the eigenfunction is correctly normalized. The squared modulus $|\phi_{Sh}|^2$ is of the form $2 + 2 \cos 2qz$ and presents oscillations (i.e. $\cos 2qz$) due to the interference between upgoing and downgoing waves. As these interferences are not taken into account in our model, we average the DOS over depth to disentangle the upgoing and downgoing waves. Reporting the result:

$$\langle |\phi_{Sh}(\mathbf{x})|^2 \rangle_z = \frac{2}{(2\pi)^3} \quad (C.4)$$

into the DOS definition yields:

$$\langle N_{Sh} \rangle_z = 2\omega \int_0^{+\infty} dq \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{2\delta(\omega^2 - \beta_0^2(q^2 + k_x^2 + k_y^2))}{(2\pi)^3}$$

$$= \frac{\omega^2}{2\pi^2 \beta_0^3}, \quad (C.5)$$

where $\langle \rangle_z$ denotes the depth average. In Equation C.5, the integral runs over positive q to

represent all possible incident (upgoing) plane Sh waves. The δ function naturally selects only those plane waves that satisfy the dispersion relation at frequency ω .

The case of P and Sv waves is more complex than the above as these two waves are coupled at the free-surface reflection. Thus, a part of the Sv DOS comes from converted P waves at the free surface and vice-versa. A P eigenmode may be written as:

$$\phi_P(\mathbf{x}) = \frac{e^{i(k_x x + k_y y)}}{(2\pi)^{3/2}} (e^{-iq_p z} \mathbf{e}^P + \dot{P} \dot{P} e^{iq_p z} \mathbf{e}_r^P + \dot{P} \dot{S} e^{iq_s z} \mathbf{e}_r^{Sv}), \quad (\text{C.6})$$

where $\mathbf{e}^P$, $\mathbf{e}_r^P$ and $\mathbf{e}_r^{Sv}$ are unit polarization vectors in the directions $(k_x, k_y, -q_p)$, (k_x, k_y, q_p) and $(-q_s, -q_s, k_x + k_y)$, respectively. The first two polarizations are longitudinal and the last one is transverse. The corresponding eigenvalue is $\lambda = \alpha_0^2(k_x^2 + k_y^2 + q_p^2)$. The vertical S wavenumber is determined by $q_s = \sqrt{\alpha_0^2(k_x^2 + k_y^2 + q_p^2)/\beta_0^2 - k_x^2 - k_y^2}$ and is always positive. For the reflection coefficients, we use the standard notations from Aki & Richards (2002). When we consider the quantity $|\phi_P(\mathbf{x})|^2$, cross terms involving P and S waves appear. Since these terms are oscillatory, they cancel out when the squared eigenfunction is averaged over depth, which in turn disentangles the P and S contributions:

$$\langle |\phi_P(\mathbf{x})|^2 \rangle_z = \frac{(1 + |\dot{P}\dot{P}|^2 + |\dot{P}\dot{S}|^2)}{(2\pi)^3} \quad (\text{C.7})$$

Eigenmodes for incident Sv waves have the form:

$$\phi_{Sv}(\mathbf{x}) = \frac{e^{i(k_x x + k_y y)}}{(2\pi)^{3/2}} (e^{-iq_s z} \mathbf{e}^{Sv} + \dot{S} \dot{S} e^{iq_s z} \mathbf{e}_r^{Sv} + \dot{S} \dot{P} e^{iq_p z} \mathbf{e}_r^P) \quad (\text{C.8})$$

where the corresponding eigenvalue is $\lambda = \beta_0^2(k_x^2 + k_y^2 + q_s^2)$, the definition of the polarization vectors is similar as above, and the vertical P wavenumber $q_p = \sqrt{\beta_0^2(k_x^2 + k_y^2 + q_s^2)/\alpha_0^2 - k_x^2 - k_y^2}$. Note that q_p may be pure imaginary when the incident angle of Sv waves is post critical for the SP conversion. However, when averaged over depth, these evanescent P contributions vanish, so that we may consider the propagating regime only. This is in line with our numerical approach where evanescent waves are neglected. The relation equivalent to Equation C.7 is given by

$$\langle |\phi_{Sv}(\mathbf{x})|^2 \rangle_z = \frac{(1 + |\dot{S}\dot{S}|^2 + |\dot{S}\dot{P}|^2)}{(2\pi)^3}. \quad (\text{C.9})$$

Let us now collect all the terms that contribute to the DOS of Sv waves. These are the incident and reflected S waves in Equation C.9 as well as the P to S conversions in Equation C.7 which

yields:

$$\begin{aligned} \langle N_{Sv} \rangle_z = & 2\omega \int_0^{+\infty} dq_s \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{\delta(\omega^2 - \beta_0^2(q_s^2 + k_x^2 + k_y^2))}{(2\pi)^3} (1 + |\dot{S}\dot{S}|^2), \\ & + 2\omega \int_0^{+\infty} dq_p \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{\delta(\omega^2 - \alpha_0^2(q_p^2 + k_x^2 + k_y^2))}{(2\pi)^3} |\dot{P}\dot{S}|^2. \end{aligned} \quad (C.10)$$

Integrating over q and using polar coordinates for the horizontal wavenumbers integrals, we get:

$$\langle N_{Sv} \rangle_z = \frac{\omega}{4\pi^2} \left(\int_0^{\omega/\beta_0} \frac{(1 + |\dot{S}\dot{S}|^2)kdk}{\beta_0^2 \sqrt{\omega^2/\beta_0^2 - k^2}} + \int_0^{\omega/\alpha_0} \frac{|\dot{P}\dot{S}|^2 kdk}{\alpha_0^2 \sqrt{\omega^2/\alpha_0^2 - k^2}} \right). \quad (C.11)$$

We now make the substitution $k \rightarrow \omega \sin j / \beta_0$:

$$\langle N_{Sv} \rangle_z = \frac{\omega^2}{4\pi^2 \beta_0^3} \left(\int_0^{\pi/2} (1 + |\dot{S}\dot{S}|^2) \sin j dj + \int_0^{j_c} \frac{\beta_0 |\dot{P}\dot{S}|^2 \sin j \cos j dj}{\alpha_0 \cos i} \right), \quad (C.12)$$

where $\sin i / \alpha_0 = \sin j / \beta_0$ and j_c is the critical angle of incidence of Sv waves for S-P conversions. We now introduce additional relations: (1) Symmetry: $\beta_0 \cos j \dot{P}\dot{S} = \alpha_0 \cos i \dot{S}\dot{P}$; (2) Energy conservation: $|\dot{S}\dot{S}|^2 + |\dot{S}\dot{P}|^2 \alpha_0 \cos i / \beta_0 \cos j = 1$ for $j \leq j_c$ and $|\dot{S}\dot{S}|^2 = 1$ for $j > j_c$. Taking these elements into account, we arrive at the result:

$$\langle N_{Sv} \rangle_z = \frac{\omega^2}{2\pi^2 \beta_0^3}. \quad (C.13)$$

A similar treatment applied to P waves gives:

$$\langle N_P \rangle_z = \frac{\omega^2}{2\pi^2 \alpha_0^3}. \quad (C.14)$$

These results generalize the theoretical equipartition ratios to the case of a halfspace with a free surface. We observe that the ratios between N_R and $\langle N_P \rangle_z$, $\langle N_{Sv} \rangle_z$ and $\langle N_{Sh} \rangle_z$ are the same as in Equations 17, 18 and 19.

APPENDIX D: PROBABILITY DISTRIBUTION OF BODY WAVE INJECTION AT DEPTH IN RAYLEIGH-TO-BODY-WAVE SCATTERING

Rayleigh waves exist simultaneously at all depths at a given time while body waves exist only at a well-defined depth. Thus in the Monte Carlo simulation, we need 2D coordinate information (i.e. x and y) to indicate the position of a Rayleigh wave and need 3D coordinate information (i.e. x , y and z) for the body-wave position. For RB scattering, the scattered body wave shares the same 2D position as the incident Rayleigh wave, but we have to add a depth (z) to the body wave (i.e. inject the body wave at a depth).

We interpret σ^{RB} as the probability distribution of RB scattering at depth. We generate

a possible depth for the scattered body wave (i.e. realizations of the distribution) using inverse transform sampling. This sampling method requires the cumulative distribution function (CDF) of σ^{RB} and a random number (*rand*) uniformly distributed from 0 to 1. We then find a depth (z_s) which satisfies

$$CDF(z_s) = \frac{\int_0^{z_s} \sigma^{RB} dz}{\int_0^\infty \sigma^{RB} dz} = rand. \quad (D.1)$$

The depth (z_s) is the scattered body-wave depth. For example, in RSh scattering (Equation 11), we write the CDF as

$$CDF(z_s) = \frac{\int_0^{z_s} \sigma_\rho^{RSh} dz}{\int_0^\infty \sigma_\rho^{RSh} dz} = \frac{\int_0^{z_s} r_1^2(z, \omega) dz}{\int_0^\infty r_1^2(z, \omega) dz}, \quad (D.2)$$

where $\frac{r_1^2(z, \omega)}{\int_0^\infty r_1^2 dz}$ is the probability distribution function (PDF) for the RSh scattering at depth (Figure D1). The main part of the PDF is distributed between the one Rayleigh-wave wavelength depth and the surface, and the CDF value is already close to 1 at the one wavelength depth. Thus the scattering depth will be mostly distributed within one wavelength from the surface. In practice, we do not compute the integral in the Monte Carlo simulations ($\int_0^{z_s} \sigma^{RB} dz$ in Equation D.1), but instead calculate the CDF at some depths (*zvec* in Algorithm 4) prior to the Monte Carlo simulation and then interpolate the depth (z) during the simulation (Algorithm 4). In the simulation, we choose the parameters about the depths as: $Dz = 0.1$ and $zmax = 10$.

APPENDIX E: GENERATING SCATTERING AZIMUTHS AND COLATITUDES

We determine the type of scattered wave based on the cross sections of all possible scattered waves, and we use the cross section of the scattered wave to determine the scattering azimuth and colatitude. In calculating a cross section, we integrate the squared scattered-wave amplitudes along all possible scattering azimuths and colatitudes (e.g. Equation 8). A scattering azimuth (colatitude) contributing more to the integral means that more scattered-wave energy will be distributed at the azimuth (colatitude), which means the scattered wave will propagate at the azimuth (colatitude) with a higher probability. Thus we interpret the integrand (e.g. in Equation 8) as the PDF of scattering azimuth (colatitude). Following the same logic in Appendix D, we use inverse transform sampling to generate scattering azimuths and colatitudes. For example, in ShR scattering, we only need the scattering azimuth and then write the PDF

Figure D1. The probability and cumulative distributions of RSh scattering with depth.

of scattering azimuth as

$$PDF(\xi_1) = \frac{\sum_m |A_{m,\rho}^{ShR}|^2}{\int_0^{2\pi} \sum_m |A_{m,\rho}^{ShR}|^2 d\xi_1} = \frac{\sin^2 \xi_1}{\int_0^{2\pi} \sin^2 \xi_1 d\xi_1} = \frac{\sin^2 \xi_1}{\pi}. \quad (E.1)$$

We observe that the scattering azimuth is more likely to be $\pi/2$ and $3\pi/2$ deg (90 and 270 degree in Figure E1a), the azimuths orthogonal to the incident wave. No scattered Rayleigh waves are expected at 0 or π (180 degree) for an incident Sh wave. These observations fit our physical expectation in Section 2.2. We calculate the CDF based on Equation E.1, generate a random number (*rand*) uniformly distributed from 0 to 1, and generate ξ_1 , where $CDF(\xi_1) = rand$. We use this same approach to generate random scattering azimuths for other scattering (e.g. the PR and SvR scattering).

For scattered body waves we need to generate both scattering azimuth and colatitude.

For example, in RSh scattering, the PDF of scattering azimuth (ξ_1) and colatitude (ψ_1) is

$$PDF(\xi_1, \psi_1) = \frac{\sum_m |A_{m,\rho}^{RSh}|^2 \sin \psi_1}{\int_0^\pi \int_0^{2\pi} \sum_m |A_{m,\rho}^{RSh}|^2 d\xi_1 d\psi_1} = \frac{\sin^2 \xi_1 \sin \psi_1}{\int_0^\pi \int_0^{2\pi} \sin^2 \xi_1 \sin \psi_1 d\xi_1 d\psi_1} = \frac{\sin^2 \xi_1 \sin \psi_1}{2\pi}, \quad (\text{E.2})$$

where $\sin \psi_1$ is due to the 2D spherical surface integrals in the total intensity of scattered Sh waves. This PDF is independent of scattering depth, and in the PDF ξ_1 and ψ_1 are independent (Figure E1b). Thus we generate the random azimuth and colatitude independently. Following the approach in last paragraph, we generate a random azimuth. Using inverse transform sampling and the PDF for the colatitude (i.e. $\sin \psi_1$), we derive that the CDF for ψ_1 is $\cos \psi_1$. Thus we generate a random angle by calculating $\cos^{-1}$ of a random number from a uniform distribution between -1 and 1.

Notice that ψ_1 and ξ_1 are not required to be independent as in RP scattering. In such a case, we need to generate a random azimuth and colatitude simultaneously. We write the PDF for the two parameters in the RP scattering as:

$$PDF(\xi_1, \psi_1, z_s) = \frac{\sum_m |A_{m,\rho}^{RP}|^2 \sin \psi_1}{\int_0^\pi \int_0^{2\pi} \sum_m |A_{m,\rho}^{RP}|^2 \sin \psi_1 d\xi_1 d\psi_1} \quad (\text{E.3})$$

$$= \frac{[r_1^2(z_s, \omega) \sin^2 \psi_1 \cos^2 \xi_1 + r_2^2(z_s, \omega) \cos^2 \psi_1] \sin \psi_1}{\int_0^\pi \int_0^{2\pi} [r_1^2(z_s, \omega) \sin^2 \psi_1 \cos^2 \xi_1 + r_2^2(z_s, \omega) \cos^2 \psi_1] \sin \psi_1 d\xi_1 d\psi_1}. \quad (\text{E.4})$$

We observe that the distribution also depends on the scattering depth (z_s , Figure E1c and E1d). In this case, we first determine z_s (Section D) and then find an azimuth and angle ($\xi_{1,s}$ and $\psi_{1,s}$) which satisfy $\int_0^{\xi_{1,s}} \int_0^{\psi_{1,s}} PDF d\xi_1 d\psi_1 = rand$ where $rand$ is a random number from a uniform distribution between 0 and 1. In practice, instead of calculating the integral ($\int_0^{\xi_{1,s}} \int_0^{\psi_{1,s}} PDF d\xi_1 d\psi_1$) in the simulations, we calculate a 2D CDF table for all possible $\xi_{1,s}$ and $\psi_{1,s}$ prior to the simulation; for a more accurate table, we use the cosine values for scattering colatitudes (i.e. $\cos \psi_1$) instead of the colatitudes (Algorithm 5). Notice that due to the cosine, we do not need to incorporate $\sin \psi_1$ in the PDF function like the one in the right end of the numerator of Equation E.4.

APPENDIX F: BODY-WAVE ANGULAR DISTRIBUTIONS ON THE FREE SURFACE

To illustrate how the free-surface boundary condition (FSBC) affects the simulation, we present the incident and reflected body-wave angular distributions on the free surface under

Figure E1. The PDFs for scattering azimuth (a) and scattering azimuth and colatitude (b, c and d). The radius in (a) is the PDF value. The color intensities in (b), (c) and (d) represent the PDF value. The black arrows represent the incident wave. The plot titles indicate the scattering type.

the mirror and mode-conversion FSBCs. Similar to Section 5.1, we divide all wave propagation angles on the free surface (up-going and down-going) into 180 equal bins on the corresponding cosine values from -1 to 1. We define the propagation angle (ψ_1) as the angle between the wave propagation direction and the down-going vertical direction (Figure 1). Thus $\cos(\psi_1)$ values for up-going/incident and down-going/reflected waves are negative and positive, respectively. At each time step of the simulation, for each type of wave (i.e. P/Sv/Sh), we count how many particles encounter the free surface and get reflected in each bin. We then calculate ratios

Algorithm 5 Calculation of a 2D CDF table

```

dazi = pi/180; dcosang = 2/180;
intg = 0; CDF = zeros(360,180);
for iazi=0:359 do
    for icosang=0:179 do
        intg = intg + PDF((iazi+0.5)*dazi,(icosang+0.5)*dcosang)* dazi * dcosang;
        CDF(iazi+1,icosang+1) = intg;
    
```

between all the particle numbers and the P-wave particle number in the vertically up-going
 bin, i.e. $\cos(\psi_1) = -1$. We average those ratios for the same wave type in a bin over a time
 range such as first and last 50 Rayleigh-wave mean free times (τ^R) in the simulation. We
 refer to those averaged ratios with respect to $\cos(\psi_1)$ as the angular distribution for each
 type of wave on the free surface (Figure F1). We observe that, in the first 50 τ^R , where
 the simulations are not yet in equipartition, the two FSBCs perform differently and lead
 to two different body-wave angular distributions (Figure F1a and F1c). However, after the
 simulations reach equipartition (Figure F1b and F1d), the incident and reflected body-wave
 distributions for the two FSBCs are identical and symmetric along the zero cosine value (i.e.
 parallel to the free surface). These symmetric body-wave angular distributions fit Lambert's
 cosine law, $|\cos(\psi_1)|$, as in the diffusion theory. The $(\alpha/\beta)^2$ for Sh/Sv waves is the intensity
 ratio between P and Sv/Sh, because we actually calculate intensity based on the number of
 particles encountering/leaving a surface, instead of energies based on the number of parti-
 cles in a space. Therefore we numerically demonstrate that the two FSBCs do not affect the
 body-wave angular distribution on the free surface in the equipartition state.

Figure F1. The body-wave angular distributions on the free surface under the mirror and mode-conversion FBSCs in the first and last 50 Rayleigh-wave mean free times. The peak in c) is due to the P-Sv-wave coupling on the free surface.