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

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5 SUMMARY

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Seismic coda waves are commonly used in estimation of subsurface Q values and monitoring subsurface changes. Coda waves mainly consist of multiply scattered 7 body and surface waves. These two types of waves interact with each other in the 8 multiple scattering process, which thus leads to a spatiotemporal evolution of the 9 body- and surface-wave energies. One cannot characterize the evolution because one 10 has not fully understood the multiple scattering of the two types of waves. Thus one 11 commonly assumes only one type of waves exists or ignores their interaction while 12 studying the coda waves. However, neglecting the interaction leads to an incorrect 13 energy evolution of the two types of waves and consequently biases the Q estima-14 tion or interpretation of coda-wave changes for monitoring. To better understand 15 the interaction between these waves during multiple scattering and to model the en-16 ergy evolution correctly, we propose a Monte Carlo algorithm to model the multiple 17 scattering process. We describe the physics of the scattering for the two types of 18 waves and derive scattering properties like cross sections for perturbations in elas-19 tic properties (e.g. density, shear modulus and Lamé parameters). Our algorithm 20

incorporates this knowledge and thus physically models the body- and surface-wave 21 energy evolution in space and time. The energy partitioning ratios between sur-22 face and body waves provided by our algorithm match the theoretical prediction 23 based on equipartition theory. In the equipartition state, our simulation results also 24 match Lambert's cosine law for body waves on the free surface. We discuss how the 25 Rayleigh-to-body-wave scattering affects the energy partitioning ratios. Our algo-26 rithm provides a new tool to study multiple scattering and coda waves in elastic 27 media with a free surface. 28

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

#### 31 1 INTRODUCTION

Coda waves are arrivals after direct waves in seismic recordings or seismic crosscorrelations. 32 One commonly uses coda waves to investigate and monitor the subsurface. By studying coda 33 waves from an earthquake event, one can estimate subsurface Q values (e.g. Aki & Chouet 34 1975). One can also compare the coda waves in two event recordings and estimate differences 35 in the coda-wave arrival times (e.g. Poupinet et al. 1984; Snieder et al. 2002; Mikesell et al. 36 2015) or waveforms (e.g. Larose et al. 2010). This method is called coda wave interferometry 37 (CWI) monitoring. By assuming the two events share a similar source location and focal mech-38 anism, one can qualitatively conclude that these differences are due to small changes of seismic 39 properties (e.g. density) in the subsurface (e.g. Snieder 2006). This monitoring method has 40 been applied to repeated event data in nature (e.g. Grêt et al. 2005) and in the lab (e.g. Larose 41 et al. 2010). This method is also commonly applied to the coda waves in seismic crosscorre-42 lations to monitor things such as the seasonal subsurface variations (e.g. Sens-Schönfelder & 43 Wegler 2006; Wang et al. 2017), volcanic eruptions (e.g. Brenguier et al. 2007, 2008), ice sheet 44 melting (e.g. Mordret et al. 2016) or the groundwater transport (e.g. Clements & Denolle 45 2018). One can further quantitatively image small changes in the subsurface from the CWI 46 monitoring results (i.e. coda-wave differences) using the physics of coda waves (e.g. Pacheco 47 & Snieder 2005; Planès et al. 2015; Margerin et al. 2016). 48

<sup>49</sup> One routinely utilizes multiply scattered waves in the coda waves in both attenuation <sup>50</sup> and CWI monitoring studies. *Multiply scattered* implies that these waves have scattered more <sup>51</sup> 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 52 requires so many simulation steps that both the computation cost and simulation result stor-53 age are prohibitively expensive. An alternative to the full-wavefield simulation is radiative 54 transfer theory, which can be used to model the spatiotemporal evolution of the seismic wave 55 energy/envelope (e.g. Wu 1985; Weaver 1990; Ryzhik et al. 1996). In the case of coupled elas-56 tic P and S waves, there exist semi-analytical solutions for the radiative transfer equations 57 in homogeneous media (e.g. Zeng 1993; Sato 1994), given the scattered-wave amplitudes are 58 isotropic. For inhomogeneous media and/or anisotropic scattering, one can adopt a Monte 59 Carlo simulation approach to solve the radiative transfer equations numerically (e.g. Gusev 60 & Abubakirov 1987; Hoshiba 1995, 1997). Furthermore, when using this approach, one only 61 needs to know the properties of scattering (e.g. scattered-wave amplitudes and mean free 62 paths) without explicitly referring to the radiative transfer equations (e.g. Margerin et al. 63 1998; Sanborn et al. 2017). 64

Most research on the radiative transfer theory so far has focused on either body or surface 65 waves, but neglected the interaction between the two. However, both body and surface waves 66 are present during the scattering process and they convert to one another via scattering (e.g. 67 Maeda et al. 2008). Thus the energy ratio between the two types of waves evolves in time 68 and space. Furthermore, Obermann et al. (2013) and Obermann et al. (2016) reveal that 69 these two waves possess different sensitivities to subsurface elastic parameters through full 70 wavefield simulations. Therefore, it is necessary to characterize the spatiotemporal evolution 71 of the energy partitioning ratio between body and surface waves, so that one can estimate 72 Q accurately or physically interpret the monitoring results (i.e. coda-wave differences). In 73 current practice, one empirically assumes the energy ratios (e.g. Obermann et al. 2019) or 74 ignores one of the two types of waves (e.g. Sens-Schönfelder & Wegler 2006; Mainsant et al. 75 2012; Obermann et al. 2015). 76

There have been previous attempts to incorporate the coupling between surface and body 77 waves within a radiative transfer framework. To incorporate this coupling into the radiative 78 transfer equations, Tregoures & Van Tiggelen (2002) considered body, Rayleigh, and Lamb 79 waves in an elastic plate with a free surface boundary condition on each surface (top and 80 bottom), where Rayleigh and Lamb waves are both a mixture of elastic body (P and S) waves; 81 Borcea et al. (2021) approximated surface waves with acoustic waves trapped in a thin layer 82 of an acoustic two-layer plate bounded by reflecting surfaces at the top and bottom. In both 83 approaches the body waves cannot leak away at depth, which is not realistic for most Earth 84 applications. Zeng (2006) introduced radiative transfer equations for coupled surface and body 85

waves by simplifying the coupling. However, these approximations and the simplification are 86 hard to justify entirely from first principles. Margerin et al. (2019) extended the conventional 87 radiative transfer equation by incorporating the coupling between surface and body waves 88 in the context of the Helmholtz equation with an impedance-type boundary condition. As 89 Margerin et al. (2019) used the scalar Helmholtz equation, only one type of body wave exists 90 in their treatment. Based on the Born approximation, Margerin et al. (2019) derived the 91 scattering mean free times for surface and body waves in a homogeneous velocity model with 92 uniformly distributed point scatterers. Margerin et al. (2019) demonstrated that the surface-93 wave scattering properties (e.g. mean free time) depend on depth, and they used a Monte 94 Carlo simulation to model the energy coupling between surface and body waves. However, a 95 significant shortcoming is that different types of body (P and S) waves can not be incorporated 96 into the simulation, because the simulation is based on the scalar equation. To overcome that 97 limitation, we take advantage of Maeda et al. (2008) who theoretically described the scattering 98 process between body and surface waves in detail. Based on these results, we derive key 99 scattering properties (e.g. cross sections and mean free time/path, Section 2), and then we use 100 these properties to develop a Monte Care simulation algorithm (e.g. Hoshiba 1991; Margerin 101 et al. 2000) to model the body- and Rayleigh-wave multiple scattering process (Section 3). 102 We focus on perturbations in density  $(\rho)$ , where these perturbations  $(\delta \rho)$  act as scatterers in 103 the media. One could extend our simulation algorithm to perturbations of P-wave and S-wave 104 velocities using Birch's Law. We conduct the simulation with and without a P-S coupling 105 free-surface boundary condition and then estimate the temporal energy ratios from multiply-106 scattered Rayleigh and body waves (Section 4). The temporal energy ratios eventually reach 107 steady values, i.e. equipartition ratios. We verify the simulation by comparing the equipartition 108 ratios to theoretical equipartition predictions. We finally discuss how to improve this algorithm 109 (Section 5). Our algorithm can improve coda-wave studies about attenuation and the use of 110 CWI for monitoring. 111

#### 112 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.

#### 125 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

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

where  $\rho_0$  is the medium density,  $\alpha_0$  is the P-wave velocity,  $\omega$  is the angular frequency and A<sup>0P</sup> 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.  $\omega$ ) here. Similarly, the intensity of a S wave is

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

where the S wave can be either Sv or Sh and  $\beta_0$  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)

$$I^{R}(\omega) = \rho_{0} U_{R} \omega^{2} (A^{0R})^{2} \int_{0}^{\infty} [r_{1}^{2}(z,\omega) + r_{2}^{2}(z,\omega)] dz, \qquad (3)$$

where  $U_R$  is the Rayleigh-wave group velocity at the frequency  $\omega$ ,  $A^{0R}$  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.

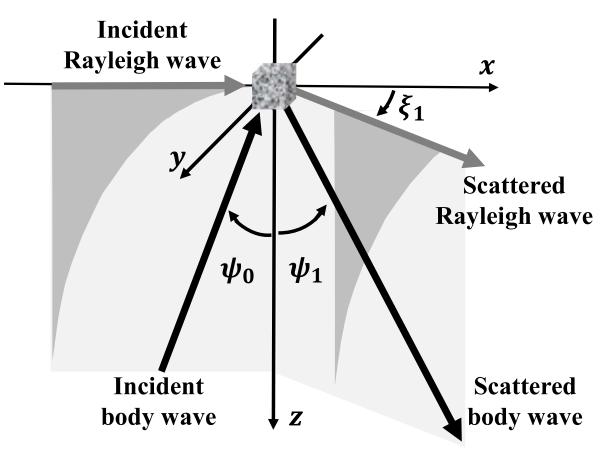


Figure 1. An illustration of single scattering process. The block is the scatterer. The thin black arrows represent local coordinate system. The thick black arrows are body waves. The gray arrows are Rayleigh waves. The gray shapes below the gray arrows represent the Rayleigh-wave eigenfunctions which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

#### <sup>147</sup> 2.2 Single scattering

The scattering cross section is defined for a single scattering, in which an incoming wave 148 encounters a scatterer, as the ratio between the energy radiated by the scatterer in all out-149 going propagation directions and the energy flux of the incoming wave. This ratio measures 150 the efficacy of the single scattering process. In elastic media, we need to calculate the cross 151 section for four types of single scattering: BR, RB, RR and BB. Calculation of each cross 152 section requires the corresponding scattering amplitude (e.g. Margerin et al. 2000). We use 153 the scattering amplitudes derived by Maeda et al. (2008) based on the Born approximation. 154 We consider scattering related to Rayleigh waves as an example in this section. 155

#### 156 2.2.1 BR scattering

<sup>157</sup> The ShR indicates a scattered Rayleigh wave from an incident Sh wave and is an example of BR <sup>158</sup> scattering. The *m*-component amplitude of a scattered Rayleigh wave due to a perturbation <sup>159</sup> of density ( $\delta \rho$ ) at  $\mathbf{x}_s$  is

$$A_{m,\rho}^{ShR}(\mathbf{x},\omega) = \int_{V} \sum_{n} G_{mn}(\mathbf{x},\mathbf{x}_{s},\omega) \omega^{2} \delta \rho A^{0Sh} e_{n}^{Sh} d\mathbf{x}_{s}.$$
 (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

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

where  $k_R = \omega/c_R$  and  $c_R$  is Rayleigh-wave phase velocity at frequency  $\omega$ .  $p_m$  is a projection 165 of the Rayleigh-wave eigenfunction  $(r_1 \text{ or } r_2)$  in the *m* direction, like  $[r_1 \cos \xi_1, r_1 \sin \xi_1, ir_2]$ , 166 where  $\xi_1$  (Figure 1) is the scattered Rayleigh-wave propagation azimuth taken from the in-167 cident wave azimuth (Snieder 1986a; Maeda et al. 2008).  $\Delta$  is the scattered Rayleigh-wave 168 travel distance from  $\mathbf{x}_s$  to  $\mathbf{x}$  along Earth's surface.  $z_s$  is the depth of perturbation  $\delta \rho$  and  $\rho_0$  is 169 the unperturbed/background density of the medium. The units of  $\delta \rho$  and  $\rho_0$  are both  $kg/m^3$ . 170 The scalar product between the polarization vectors in Equation 4  $(\sum p_n^* e_n^{0Sh})$  determines 171 the coupling between the incident Sh and scattered Rayleigh waves. As "the incident Sh wave 172 only possesses a horizontal component in the y direction (n = 2),  $\sum_{n} p_n^* e_n^{0Sh}$  becomes  $p_2^*$ , i.e. 173  $r_1 \sin \xi_1$ . We then rewrite Equation 4 as 174

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

In Equation 6, we remark that the scattered Rayleigh-wave amplitude does not depend on the 175 incident Sh wave angle  $(\psi_0)$ . Instead, we observe that the Rayleigh-wave amplitude depends 176 on the Rayleigh-wave propagation azimuth  $(\xi_1)$ , and this observation offers physical insights 177 into the scattering process. For example, if the scattered Rayleigh wave follows the same 178 azimuth as the incident wave  $(\xi_1 = 0)$ , we have  $\sin \xi_1 = 0$  and as a consequence, the scattered 179 amplitude is 0, which implies the absence of the ShR conversion in the forward direction. This 180 result, sometimes termed as selection rule, fits our physical intuition. An incident Sh wave 181 with particle motion in y direction does not excite a Rayleigh-wave propagating in x direction 182

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<sup>183</sup> because the two directions are orthogonal; furthermore, among all azimuths, the strongest
<sup>184</sup> excitation of Rayleigh waves occurs in the Sh wave polarization direction, i.e. the y direction.
<sup>185</sup> We next assume that the size of the density perturbation is negligible compared to the
<sup>186</sup> Rayleigh-wave wavelength and further simplify Equation 6. Thus, we are in the so-called
<sup>187</sup> Rayleigh scattering regime (e.g. Wu & Aki 1985) and can rewrite Equation 6 as

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

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:

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

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

<sup>191</sup> 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 <sup>192</sup> total energy depends on the scatterer depth,  $z_s$ . Based on the definition of the scattering cross <sup>193</sup> section, we write the ShR cross section as

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

#### 198 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

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

Notice the unit for  $\sigma_{\rho}^{RSh}$  is m, instead of  $m^2$  like  $\sigma_{\rho}^{ShR}$ . 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:

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

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.

#### 209 2.3 Isotropic incident angle assumption

Some cross sections are dependent on the incident angle,  $\psi_0$  (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  $\sigma_{\rho}^{PR}$ depends on the incident angle ( $\psi_0$ ), and we derive the cross section by following the same steps as in Section 2.2:

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

<sup>215</sup> 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 <sup>216</sup> (Equation 10) except the different incident wave velocities. We write  $C = r_1^2 \sin^2 \psi_0 + 2r_2^2 \cos^2 \psi_0$ <sup>217</sup> and note that this term, similar to  $r_1^2$  in Equation 10, determines the coupling between the <sup>218</sup> incident P and scattered Rayleigh waves. For example,  $\psi_0 = 0$  (a vertically incident P-wave) <sup>219</sup> and  $\psi_0 = \pi/2$  (a horizontally incident P-wave) lead to purely vertical ( $C = 2r_2^2$ ) and horizon-<sup>220</sup> tal ( $C = r_1^2$ ) coupling, respectively. Therefore the PR cross section dependence on  $\psi_0$  makes <sup>221</sup> 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 an-222 gle. This involvement significantly complicates any simulation, especially the following Monte 223 Carlo simulation, because we need to calculate the BR cross section for a given incident angle 224  $(\psi_0)$  and use the new cross section to determine scattering Rayleigh-wave azimuths  $(\xi_1)$ . Fur-225 thermore, numerical simulations (e.g. Paul et al. 2005) demonstrate that the incident angles 226 become evenly distributed on the unit sphere (i.e. isotropic) after a sufficiently large number of 227 scattering events. Thus, we can eliminate the incident angle dependence of the BR scattering 228 cross sections (e.g.  $\sigma_{\rho}^{PR}$ ) by averaging the cross sections over the incident angles ( $\psi_0$ ): 229

$$\widetilde{\sigma}_{\rho}^{PR} = \frac{1}{\int_{0}^{\pi} \sin\psi_{0} d\psi_{0}} \int_{0}^{\pi} \sigma_{\rho}^{PR} \sin\psi_{0} d\psi_{0} = \frac{\omega^{3}}{12\alpha_{0}c_{R}U_{R}\int(r_{1}^{2}+r_{2}^{2})dz} (r_{1}^{2}+r_{2}^{2})V^{2} \left(\frac{\delta\rho}{\rho_{0}}\right)^{2}.$$
 (14)

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

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#### 232 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

$$l^w = \frac{1}{n\sigma^w},\tag{15}$$

where  $\sigma^w$  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  $(\tau^w)$  is defined as

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

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.  $\sigma_{\rho}^{ShR}$  and  $\sigma_{\rho}^{Sh}$ ). This depth dependence is related to the coupling of body and Rayleigh waves.

#### 252 2.5 Theoretical equipartition value

We can calculate the theoretical equipartition energy ratio between two types of multiplyscattered 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-

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<sup>258</sup> scattered body and Rayleigh waves as

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

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

$$\bar{\bar{E}}_{R} = \int_{0}^{\infty} \frac{\tau_{\rho}^{RSh}(\omega)}{\tau_{\rho}^{ShR}(z_{s},\omega)} dz_{s} = \int_{0}^{\infty} \frac{\sigma_{\rho}^{ShR}(z_{s},\omega)\beta_{0}}{\sigma_{\rho}^{RSh}(\omega)U_{R}} dz_{s} = \frac{\pi\beta_{0}^{3}}{\omega c_{R}U_{R}},$$
(19)

where  $\overline{E}_R$  is the total Rayleigh-wave energy over the whole medium, and  $\overline{E}_P$  is an integral of Pwave energy over a constant-depth plane and thus is the energy density at the depth. The bodywave 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.

#### 273 **3 MONTE CARLO SIMULATION**

We simulate multiple scattering with a Monte Carlo method. The Monte Carlo simulation 274 method has been applied to multiply scattered acoustic/elastic body waves (e.g. Hoshiba 1991; 275 Margerin et al. 2000). We use this method to simulate multiply-scattered body and Rayleigh 276 waves in a statistically uniform isotropic elastic medium filled with point scatterers. The idea 277 underlying the Monte Carlo simulation is to simulate the propagation and scattering of wave 278 energy as a random walk for a particle and repeat the random walk N times independently 279 (Algorithm 1). After the N simulations, we count how many body and Rayleigh particles exist 280 at each time step and interpret the body and Rayleigh particle numbers as the body- and 281 Rayleigh-wave energy, respectively. Furthermore, by discretizing the 3D medium into a grid 282 and recording changes of the particle numbers at each grid cell with time, we estimate the 283 evolution of wave energy in time and space. 284

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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.

#### 290 3.1 Initialization

We launch a particle at the source location in the beginning of one simulation. The particle 291 can be a body (P/Sv/Sh) or Rayleigh wave (Algorithm 2). We can model different source 292 mechanisms by changing initial wave types (e.g. Margerin et al. 2000) and propagation direc-293 tions (i.e. azimuth and colatitude). For example, if the source is an explosion, we can set that 294 only P waves are generated at the source location. The P-wave initial azimuths are randomly 295 generated with a uniform probability distribution between 0 and  $2\pi$ , and the cosines of the 296 P-wave initial colatitudes are randomly generated from a uniform distribution between -1 297 and 1 (Algorithm 2). For a shear-force source like a fault, all types of waves are randomly 298 selected in proportions equal to their respective radiated energy. Based on the initial wave 299 type, we compute a random free time (T) which indicates the travel time before the next 300 scattering happens. We will cover the details of free time in the next section (Section 3.2). 301 We also calculate the wave propagation vector  $(k_x, k_y, k_z)$  based on the propagation azimuths 302 and colatitudes. 303

#### <sup>304</sup> **3.2** Effective cross section and mean free time

The initialized particle propagates during the random free time T. We compute T as T =305  $-\tau^w \ln(rand)$  where rand is a random number with a uniform probability distribution from 306 0 to 1 (e.g. Hoshiba 1991), and w indicates a body (B) or Rayleigh wave (R). We directly 307 follow the computation for Rayleigh-wave free time but not for the body-wave. Calculation 308 of the body-wave free time between two scattering events is not straightforward, since the 309 body-wave mean free time ( $\tau^B$  e.g.  $\tau_{\rho}^{Sh}$ ) varies with depth (Section 2.4). This is because 310  $\tau_{\rho}^{Sh}$  is inversely proportional to  $\sigma_{\rho}^{Sh}$ , where  $\sigma_{\rho}^{Sh}$  includes the depth-dependent  $\sigma_{\rho}^{ShR}$ . Thus, 311 calculation of the body-wave free time requires tracking of the body-wave depth in order to 312 integrate the variation of the mean free time in the propagation. To address this difficulty, we 313 adopt a trick called delta collisions (Lux & Koblinger 1991). The idea of delta collisions is to 314 impose an effective and constant cross section ( $\sigma^{Be}$  where e stands for 'effective') and mean 315 free time. To compensate for the difference between  $\sigma^{Be}$  and the real cross section at a given 316

Algorithm 1 Monte Carlo simulation algori				
$\sigma^{Be} = \sum_{B'} \sigma^{BB'} + max[\sigma^{BR}(z)]$	$\triangleright$ Calculating effective body-wave cross section			
$\triangleright B$ and $B'$ can be an	y possible body wave in scattering, P, Sv or Sh			
$\tau^{Be} = 1/n/\sigma^{Be}/vb$	$\triangleright$ Effective body-wave mean free time			
$\sigma^R = \sigma^{RR} + \sum_{B} \sigma^{RB}$	$\triangleright$ Rayleigh wave cross section			
$\tau^R = 1/n/\sigma^R / vr$	$\triangleright$ Rayleigh wave mean free tim			
Set dt, the time step for recording particle	numbers for each wave mode, P, Sv, Sh and F			
for $i = 1 : N$ th simulation <b>do</b>				
[mode T azi0 kx ky kz] = Initialization	() $\triangleright$ Wave mode, free time, propagatio			
azimuth and vector				
Set x, y and z at the source location				
$\mathbf{while} \text{ itime} < \text{Nstep } \mathbf{do}$	$\triangleright$ <i>i</i> th simulation start			
$\mathbf{if} \ \mathbf{mode} == \mathbf{B} \ \mathbf{then}$	▷ Body-wave propagatio			
if $T > $ deltat <b>then</b>	$\triangleright$ No scattering happe			
x = x + deltat*vb*kx; y = y +	-deltat*vb*ky; z = z+deltat*vb*kz			
$\mathbf{if} \ \mathbf{z} < 0 \ \mathbf{then}$	$\triangleright$ Encounter the free surface			
FreeSurfaceBoundaryCon	dition			
itime = itime + 1	$\triangleright$ Record body-wave type at this time point			
T = T - deltat				
deltat = dt				
else	$\triangleright$ A scattering will happe			
$\mathbf{x} = \mathbf{x} + T^* \mathbf{v} \mathbf{b}^* \mathbf{k} \mathbf{x}; \ \mathbf{y} = \mathbf{y} + T^* \mathbf{v}$	$b^*ky; z = z + T^*vb^*kz$			
$\mathbf{if}  \mathbf{z} < 0  \mathbf{then}$	$\triangleright$ Encounter the free surface			
FreeSurfaceBoundaryCon	dition			
deltat = deltat - T				
[mode T azi0 kx ky kz] = sca	$atterb(azi0)$ $\triangleright$ Body-wave scattering			
$\mathbf{if} \ \mathrm{mode} == \mathrm{R} \ \mathbf{then}$	▷ Rayleigh-wave propagation			
if $T > $ deltat <b>then</b>	$\triangleright$ No scattering happe			
$x = x + deltat^*vr^*kx; y = y +$	deltat*vr*ky			
	▷ Record Rayleigh wave type at this time poin			
T = T - deltat				
deltat = dt				
else	$\triangleright$ A scattering will happe			
$\mathbf{x} = \mathbf{x} + T^* \mathbf{v} \mathbf{r}^* \mathbf{k} \mathbf{x}; \ \mathbf{y} = \mathbf{y} + T^* \mathbf{v}$	r*ky			
deltat = deltat - T				

Generate a particle; its <b>mo</b>	de can be a body $(B = P/Sv/Sh)$ or Rayleigh (R) wave
$\mathbf{if} \ \mathbf{mode} == \mathbf{B} \ \mathbf{then}$	
$T = -\tau^{Be} * \ln(rand)$	$\triangleright$ Generate a random free time from a random number
ang = acos(-1+2*rand)	▷ A random colatitude in $[0,\pi]$
azi0 = 2*pi*rand	$\triangleright$ A random propagation azimuth in $[0,2\pi]$
kx = sin(ang)*cos(azi0)	$\triangleright$ 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)	$\triangleright$ 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 - prsin Algorithm 3) between  $\sigma^{Be}$  and  $\sigma^{B}(z)$ . The imaginary scattering does not change the bodywave propagation direction. Notice that we do not need to introduce the effective mean free time for Rayleigh waves because both  $\overline{\sigma}^{RB}$  and  $\overline{\sigma}^{RR}$  (e.g. Equation 12) are independent of depth.

#### 323 3.3 Scattering

After propagating for time T, the particle encounters a scatterer/perturbation, and scattering 324 occurs. We generate a uniformly distributed random value in the range [0, 1] to simulate all 325 possible conversions and determine the scattered wave type (Algorithms 3 and 4). Notice that 326 for incident Rayleigh particles, if a RB conversion happens, we re-inject the scattered body 327 particle at a depth based on the distribution of  $\sigma^{RB}$  as a function of depth (Appendix D). 328 We generate the scattering azimuths and colatitudes  $(\xi_1 \& \psi_1 \text{ in Section 2 or azi } \& ang in the$ 329 pseudocode) of scattered waves based on the probabilistic interpretation of scattering cross 330 sections (Appendix E). We add the scattering azimuths to the incident azimuth to achieve 331 the propagation azimuth. Due to the isotropic incident angle assumption (Section 2.3), we do 332 not need the incident angles in this part. We discuss this assumption in Section 5.1. Based on 333

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)  $\sigma^B(z) = \sigma^{BR}(z) + \sum\limits_{B'} \sigma^{BB'}$  $\triangleright$  Cross section for all possible scattering at this depth  $prs = \sigma^B(z)/\sigma^{Be}$ ▷ 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  $\triangleright$  scattered P wave, B' = Pmode = Pif  $\sigma^{BP}/\sigma^B(z) < rand < (\sigma^{BP} + \sigma^{BSv})/\sigma^B(z)$  then ▷ Possibility for BSv scattering  $\triangleright$  scattered Sv wave, B' = Svmode = Svif  $(\sigma^{BP} + \sigma^{BSv})/\sigma^B(z) < rand < (\sigma^{BP} + \sigma^{BSv} + \sigma^{BSh})/\sigma^B(z)$  then ▷ Possibility for BSv scattering mode = Sh $\triangleright$  scattered Sh wave, B' = Sh $T = -\tau^{B'e} * \ln(rand)$ ▷ Generate a random free time from a new random number Generating azi and ang based on probability distributions (Appendix E) azi0 = azi0 + azikx = sin(ang)\*cos(azi0)▷ 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 + azikx = cos(azi0)▷ Rayleigh-wave propagation vector in Cartesian coordinates ky = sin(azi0)else ▷ 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: [mode T azi0 kx ky kz z] = scatterr(azi0) zvec = 0 : Dz : zmax $\triangleright$  The depth vector, from 0 to zmax, for injecting body wave if  $rand < \sigma^{RR} / \sigma^{R}$  then  $\triangleright$  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 + azikx = cos(azi0)▷ Rayleigh-wave propagation vector in Cartesian coordinates ky = sin(azi0)else  $\triangleright$  RB scattering if  $rand < (\sigma^{RR} + \sigma^{RP})/\sigma^{R}$  then  $\triangleright$  RP scattering, B = Pmode = Pif  $(\sigma^{RR} + \sigma^{RP})/\sigma^R < rand < (\sigma^{RR} + \sigma^{RP} + \sigma^{RSv})/\sigma^R$  then  $\triangleright$  RSv scattering, B = Svmode = Svif  $(\sigma^{RR} + \sigma^{RP} + \sigma^{RSv})/\sigma^R < rand$  then mode = Sh $\triangleright$  RSv scattering, B = Sh $z = interp1(\sigma^{RB}(zvec) / \int \sigma^{RB}(z) dz, zvec, rand)$  $\triangleright$  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 + azikx = sin(ang)\*cos(azi0)▷ Body-wave propagation vectors in Cartesian coordinates ky = sin(ang)\*sin(azi0)kz = cos(ang);

#### 336 3.4 Boundary conditions

We assume the free surface is flat and adopt two types of free-surface boundary conditions 337 (FSBCs) in the simulation: mirror-like reflection and mode conversion. The mirror FSBC con-338 serves the wave energy and propagation vector except for the sign of the vertical component. 339 This FSBC does not modify the incident wave type (i.e. no mode conversion). The mode-340 conversion FSBC allows the wave mode conversion (i.e. P to Sv or Sv to P) based on energy 341 reflection coefficients. Depending on the incident-wave angle and wave type (B=P/Sv), we 342 can calculate the corresponding reflection coefficient  $(R_{BB})$  for a reflected wave remaining as 343 the same wave type (e.g. Aki & Richards 2002, Chapter 5.2.2).  $R_{BB}$  is the reflected wave 344

amplitude ratio relative to the incident-wave amplitude. Given the incident-wave intensity is 345 1, we recognize that the square of the coefficient  $(R_{BB}^2)$  is the intensity of the reflection wave 346 and the probability of this reflection. We then generate a random number from a uniform 347 distribution between 0 and 1. If the random number is less than or equal to  $R_{BB}^2$ , no mode 348 conversion happens; otherwise, the incident P or Sv wave will convert to a Sv or P wave, re-349 spectively. If the mode conversion happens, we also recalculate the free time for the reflected 350 waves. For the boundary condition in the depth, we assume that body waves can propagate 351 to infinite depth in the simulations. 352

#### 353 4 SIMULATION RESULTS

We set the frequency be 1 Hz and choose the medium parameters as follows:  $\alpha_0=5$  km/s, 354  $\beta_0=3$  km/s and thus  $c_R=2.74$  km/s. We set the medium to be 10 km (zmax in Algorithm 4) 355 thick. We assume that there is no intrinsic attenuation in the medium, which means that the 356 seismic-wave energy will not irreversibly convert to other types of energies. We also assume 357 that the scatterers  $(\delta \rho)$  are randomly distributed in the medium, and set the perturbation 358 density relative to the background  $(\delta \rho / \rho_0)$  to 0.2 and a scatterer volume (V) to be 0.5 m<sup>3</sup>. We 359 also set the volume density of scatterers (n) equal to  $1 m^{-3}$ . We compute the Rayleigh-wave 360 eigenfunctions based on these velocities (Appendix A) and calculate all the cross sections and 361 mean free times (Appendix B and Equation 16). The Rayleigh-wave mean free path  $(l^R)$  is 362 35.8 km (Equation 15) and is of the same order of mean free path as in Earth's crust (e.g. 363 Margerin et al. 1999). Note that the ratio between  $l^R$  and the Rayleigh-wave wavelength 364 (2.74 km) is 13 and fulfills the condition of application of radiative transfer theory that the 365 mean free path should be much larger than the corresponding wavelengths (e.g. Ryzhik et al. 366 1996). In the simulation, we place a source at 1 km depth. The source emits P and Rayleigh 367 waves/particles. During the random walk for one particle, we record the location and mode 368 for the particle every 1 s (dt in Algorithm 1). The random walk lasts 3000 s (Nstep=3000 in 369 Algorithm 1). We repeat the random walk 100 million  $(N = 10^8)$  times. For each wave mode, 370 we count the particles in a certain space (e.g. the shallowest 1km depth of the medium) in all 371 the random walks and then divide the particle number with N to get the wave energy. 372

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

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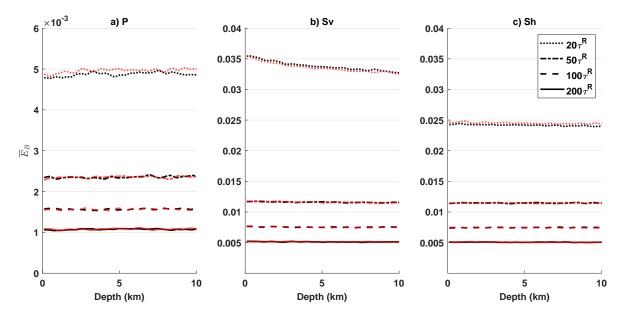


Figure 2. The simulated body-wave energy densities as a function of depth. We plot the energy densities at different simulation time in the unit of Rayleigh-wave mean free time ( $\tau^R$ ): 20, 50, 100 and 200  $\tau^R$ . The black curves are from the simulation with the mirror free surface boundary 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  $(\overline{\overline{E}}_R)$  by counting the number of Rayleigh waves in the whole medium. We observe that the energy ratios between  $\overline{\overline{E}}_R$  and  $\overline{E}_{Sv/h}$  become homogeneous after 50  $\tau^R$ , and the energy ratios between  $\overline{\overline{E}}_R$  ( $\overline{E}_{Sv/h}$ ) and  $\overline{E}_P$  become constant after 100  $\tau^R$  (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 384 simulation, similar to the last one, we observe homogeneous body-wave energies in depth 385 in the equipartition stage (Figure 2). This mode-conversion FSBC provides similar energy 386 partition ratios among Rayleigh and body waves compared to the mirror FSBC simulation 387 (Figure 4 and Table 1). This similarity is not surprising because Trégourès & van Tiggelen 388 (2002) theoretically demonstrated that the mode-conversion (i.e traction free) FSBC does 389 not affect the body-wave energy partition ratios. Here we numerically demonstrate that no 390 matter which FSBC is used, the simulation reaches equipartition. In addition, the body-wave 391 angular distributions on the free surface match Lambert's cosine law from the diffusion theory 392 (Appendix F). 393

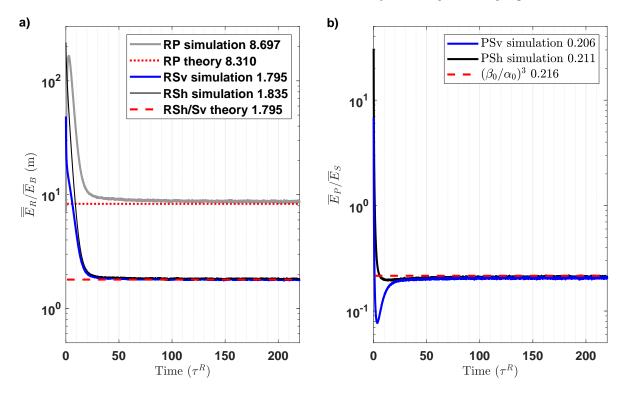
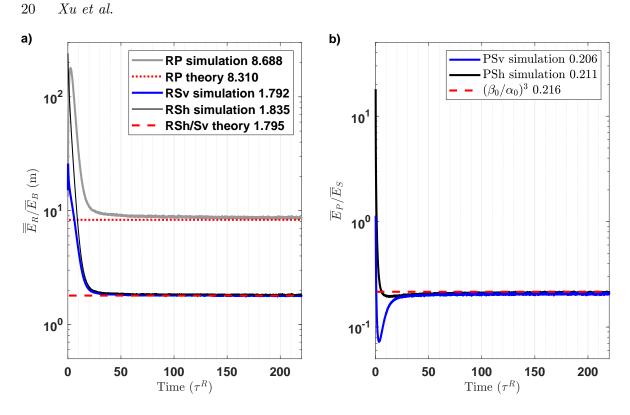


Figure 3. Temporal evolution of the energy partitioning ratios among Rayleigh, P, and Sv/h waves in the simulation with the mirror FSBC. We estimate  $\overline{E}_B$  in the shallowest 1 km depth of the medium. We calculate the simulated energy ratio from the last 50  $\tau^R$  simulation results. The 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.

#### 394 5 DISCUSSION

#### 395 5.1 Body-wave incident angles

We average the incident-angle-dependent cross sections by assuming that the incident body 396 waves are isotropic, i.e. evenly distributed on a unit sphere. We examine this assumption 397 here using our simulation results. We discuss the scattering colatitudes ( $\psi_1$  in Figure 1) 398 because we actually use the colatitudes in simulation of the wave propagation (e.g.  $cos(\psi_1)$ ). 399 If the scattered-body-wave colatitudes are isotropic,  $\cos(\psi_1)$  will be equal to 1 for all incident 400 angles and the incident angles will also be isotropic. The positive and negative cosine values 401 represent down-going and up-going wave propagation, respectively. We divide the potential 402 range for  $\cos(\psi_1)$ , from -1 to 1, into 180 even bins. At each time step in the simulation, we 403 count the particle (i.e. wave) numbers for all types of body waves in each bin from the 404 free surface to 10 km depth; we then calculate ratios between the particle numbers and 405 the mean of the P particle numbers in all the bins. We finally average the ratios in a time 406



**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.

<sup>407</sup> range when the energy partitioning ratios are stable, such as the last 50 Rayleigh-wave mean <sup>408</sup> free times (50  $\tau^R$ ). We refer to these averaged ratios with respect to  $\cos(\psi_1)$  as angular <sup>409</sup> distributions for each type of wave (Figure 5). Based on the isotropic angular distributions, <sup>410</sup> we expect the P- and Sv-/Sh-wave ratios to be 1 and  $(\alpha_0/\beta_0)^3$ , respectively. In the two <sup>411</sup> 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. 418 First, we check the body-wave angular distributions when we only have body-wave scattering 419 in the simulation. To do that, we turn off the coupling between body and Rayleigh waves, 420 i.e. no RB or BR scattering. We then run this modified simulation with the mode-conversion 421 FSBC and calculate the angular distributions as above. We observe that all the body-wave 422 angular distributions are isotropic after the simulation reaches equipartition (Figure 5c). This 423 observation fits the generalized diffusion theory for the mode-conversion FSBC (e.g. Trégourès 424 & van Tiggelen 2002) and indicates that the biases are not related to body-wave multiple scat-425 tering. Second, we turn on the Rayleigh-wave coupling and require the RP and RSv scattering 426 colatitudes to be isotropic while the RSh scattering is already isotropic from the physics (Fig-427 ure 5d). We observe that this new simulation also generates isotropic distributions for all 428 body waves. Furthermore, this new simulation provides more accurate energy equipartition 429 ratios than the two in Section 4 (Figure 6 and Table 1). Thus, we conclude that the biases 430 in the body-wave angular distributions in the simulation algorithm are due to the anisotropic 431 RP and RSv scattering colatitude patterns. The isotropic scattering patterns can be used 432 in the multiple scattering simulations as done before (e.g. Sato & Nishino 2002). However, 433 the anisotropic RP and RSv scattering patterns are from the physics and change with depth 434 (Figure E1). Therefore this observation and these biases need to be further investigated and 435 more fully understood. This is a new observation that has not been noted in the literature 436 before. 437

#### 438 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

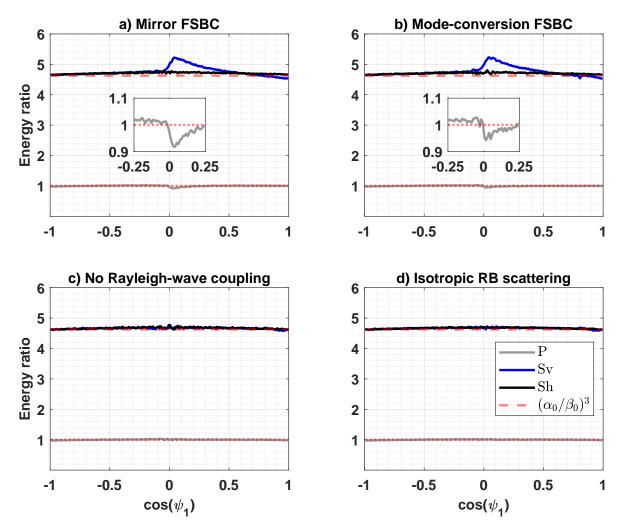


Figure 5. The body-wave angular distributions from the simulation with the mirror FSBC (a), the mode-conversion FSBC (b), the mode-conversion FSBC and no RB or BR scattering (c), and the mode-conversion FSBC and isotropic RB scattering (d). We use anisotropic RB scattering in (a) and (b). The theoretical 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 445 theory or Monte Carlo simulations yet. We do not consider complex subsurface media such 446 as lateral heterogeneities (e.g. Yu et al. 2021), interfaces (e.g. Margerin et al. 1998; Sanborn 447 et al. 2017), a topographic free surface (e.g. Snieder 1986b; Takemura et al. 2015; Wang et al. 448 2015) or intrinsic attenuation (e.g. Zhang et al. 2021) into our simulations yet. Incorporating 449 those into our algorithm is a promising direction for future studies and thus help studies like 450 surface waves in microseisms (e.g. Ziane & Hadziioannou 2019; Gualtieri et al. 2020) 451 We model Sv and Sh waves separately in our algorithm. However, in practice, S waves are 452

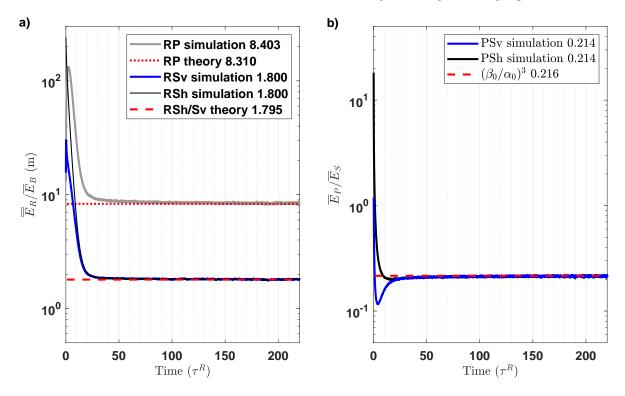


Figure 6. Temporal evolution of the energy partitioning ratios among Rayleigh, P and Sv/h waves in the simulation with the mode-conversion FSBC and isotropic RB scattering. All data processing and figure settings match those in Figure 3.

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.

#### 459 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-

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date the algorithm by comparing the simulation results to the theoretical energy ratios. We 467 numerically demonstrate that the simulations with the mirror and mode-conversion free sur-468 face boundary conditions provide similar energy equipartition ratios close to the theoretical 469 equipartition values. In the equipartition state, the body-wave angular distributions on the 470 free surface match Lambert's cosine law under the two different free surface boundary condi-471 tions. Our results also indicate that biases in the simulation results are due to the anisotropic 472 BR scattering angle patterns. Our research provides a new tool to study the multiple scatter-473 ing phenomena in elastic media, and thus may aid coda wave studies such as Q estimation or 474 interpretation of coda-wave monitoring results. 475

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#### 484 8 DATA AVAILABILITY

<sup>485</sup> The data underlying this article are available in the article.

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#### 632 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  $\omega$  and depth z as

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

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

where  $r_1$  and  $r_2$  are the eigenfunctions,  $k_R$  is the Rayleigh-wave wavenumber, and  $\Delta$  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 637 analytical expressions for the eigenfunctions are

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

638 and

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

<sup>639</sup> We calculate the eigenfunctions for the velocity model where  $\alpha_0=5$  km/s and  $\beta_0=3$  km/s <sup>640</sup> (Figure A1), and we use the eigenfunctions in the scattering amplitudes (e.g. Equation 7) and <sup>641</sup> cross sections (e.g. Equation 10).

#### **APPENDIX B: SCATTERING CROSS SECTIONS**

#### 643 B1 Body-to-Rayleigh-wave cross sections

<sup>644</sup> For scattering due to perturbations in the Lamé parameter (i.e.  $\delta\lambda$ ),

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

$$\sigma_{\lambda}^{SvR} = \sigma_{\lambda}^{ShR} = 0. \tag{B.2}$$

For  $\delta \rho$  scatters,

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

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

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

where  $\psi_0$  is the body-wave incident angle (Figure 1). After averaging over incident angles,

$$\widetilde{\sigma}_{\rho}^{PR} = \frac{1}{\int_{0}^{\pi} \sin(\psi_{0}) d\psi_{0}} \int_{0}^{\pi} \sigma_{\rho}^{PR} \sin(\psi_{0}) d\psi_{0} = \frac{\omega^{3}}{12\alpha_{0}c_{R}U_{R}\int(r_{1}^{2} + r_{2}^{2}) dz} (r_{1}^{2} + r_{2}^{2}) V^{2} \left(\frac{\delta\rho}{\rho_{0}}\right)^{2},$$
(B.6)

$$\widetilde{\sigma}_{\rho}^{SvR} = \frac{1}{\int_{0}^{\pi} \sin(\psi_{0}) d\psi_{0}} \int_{0}^{\pi} \sigma_{\rho}^{SvR} \sin(\psi_{0}) d\psi_{0} = \frac{\omega^{3}}{24\beta_{0}c_{R}U_{R} \int (r_{1}^{2} + r_{2}^{2}) dz} (r_{1}^{2} + 4r_{2}^{2}) V^{2} \left(\frac{\delta\rho}{\rho_{0}}\right)^{2},$$
(B.7)

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

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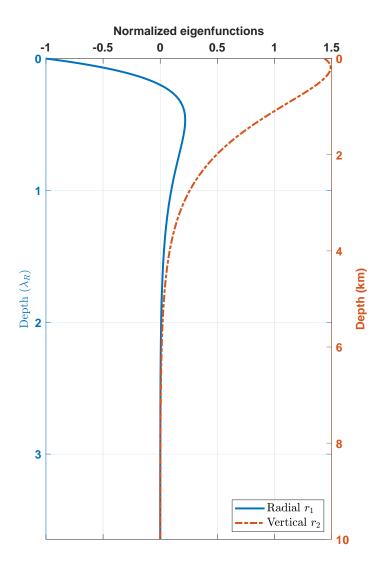


Figure A1. Radial  $(r_1)$  and vertical  $(r_2)$  eigenfunctions vary with depth at 1 Hz. The eigenfunction values are normalized by the absolute value of  $r_1$  at the free surface (z = 0). The depth axes are Rayleigh-wave wavelength  $(\lambda_R)$  and kilometers to demonstrate how shallow scatterers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

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

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$$\begin{split} \sigma_{\mu}^{PR} &= \frac{\omega^{3}\beta_{0}^{4}}{8\alpha_{0}^{3}c_{R}U_{R}^{3}\int(r_{1}^{2}+r_{2}^{2})dz} \left[ 3r_{1}^{2}\sin^{4}(\psi_{0}) + \frac{8}{k_{R}^{2}}\left(\frac{\partial r_{2}}{\partial z}\right)^{2}\cos^{4}(\psi_{0}) + \frac{8r_{1}}{k_{R}}\frac{\partial r_{2}}{\partial z}\sin^{2}(\psi_{0})\cos^{2}(\psi_{0}) \right. \\ &\left. + \frac{1}{k_{R}^{2}}\left(\frac{\partial r_{1}}{\partial z}\right)^{2}\sin^{2}(2\psi_{0}) + r_{2}^{2}\sin^{2}(2\psi_{0}) - \frac{2}{k_{R}}\frac{\partial r_{1}}{\partial z}r_{2}\sin^{2}(2\psi_{0})\right] V^{2}\left(\frac{\delta\mu}{\mu_{0}}\right)^{2}, \quad (B.9) \\ \sigma_{\mu}^{SvR} &= \frac{\omega^{3}\beta_{0}}{8c_{R}U_{R}^{3}\int(r_{1}^{2}+r_{2}^{2})dz} \left[ \frac{3}{4}r_{1}^{2}\sin^{2}(2\psi_{0}) + \frac{2}{k_{R}^{2}}\left(\frac{\partial r_{2}}{\partial z}\right)^{2}\sin^{2}(2\psi_{0}) - \frac{2}{k_{R}}r_{1}\frac{\partial r_{2}}{\partial z}\sin^{2}(2\psi_{0}) \right. \\ &\left. + r_{2}^{2}\cos^{2}(2\psi_{0}) + \frac{1}{k_{R}^{2}}\left(\frac{\partial r_{1}}{\partial z}\right)^{2}\cos^{2}(2\psi_{0}) - \frac{2}{k_{R}}\frac{\partial r_{1}}{\partial z}r_{2}\cos^{2}(2\psi_{0})\right] V^{2}\left(\frac{\delta\mu}{\mu_{0}}\right)^{2}, \quad (B.10) \\ \sigma_{\mu}^{ShR} &= \frac{\omega^{3}\beta_{0}}{8c_{R}U_{R}^{3}\int(r_{1}^{2}+r_{2}^{2})dz} \left[ r_{1}^{2}\sin^{2}(\psi_{0}) + r_{2}^{2}\cos^{2}(\psi_{0}) + \frac{1}{k_{R}^{2}}\left(\frac{\partial r_{1}}{\partial z}\right)^{2} - \frac{2}{k_{R}}\frac{\partial r_{1}}{\partial z}r_{2}\cos(\psi_{0}) \right] V^{2}\left(\frac{\delta\mu}{\mu_{0}}\right)^{2} \right] V^{2}\left(\frac{\delta\mu}{\mu_{0}}\right)^{2} \\ (B.11) \end{split}$$

648 After averaging over incident angles,

$$\widetilde{\sigma}_{\mu}^{PR} = \frac{\omega^{3}\beta_{0}^{4}}{15\alpha_{0}^{3}c_{R}U_{R}^{3}\int(r_{1}^{2}+r_{2}^{2})dz} \left[3r_{1}^{2}+\frac{3}{k_{R}^{2}}\left(\frac{\partial r_{2}}{\partial z}\right)^{2}+\frac{2r_{1}}{k_{R}}\frac{\partial r_{2}}{\partial z}+\frac{1}{k_{R}^{2}}\left(\frac{\partial r_{1}}{\partial z}\right)^{2}+r_{2}^{2}-\frac{2}{k_{R}}\frac{\partial r_{1}}{\partial z}r_{2}\right]V^{2}\left(\frac{\delta\mu}{\mu_{0}}\right)^{2},$$
(B.12)

$$\begin{split} \widetilde{\sigma}_{\mu}^{SvR} = & \frac{\omega^{3}\beta_{0}}{c_{R}U_{R}^{3}\int(r_{1}^{2}+r_{2}^{2})dz} \left[ \frac{r_{1}^{2}}{20} + \frac{2}{15k_{R}^{2}} \left( \frac{\partial r_{2}}{\partial z} \right)^{2} - \frac{2}{15k_{R}}r_{1}\frac{\partial r_{2}}{\partial z} + \frac{7}{120}r_{2}^{2} + \frac{7}{120k_{R}^{2}} \left( \frac{\partial r_{1}}{\partial z} \right)^{2} - \frac{7}{60k_{R}}\frac{\partial r_{1}}{\partial z}r_{2} \right] V^{2} \left( \frac{\delta\mu}{\mu_{0}} \right)^{2}, \end{split}$$
(B.13)

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

#### 649 B2 Rayleigh-to-body-wave cross sections

<sup>650</sup> For perturbations in the Lamé parameter  $(\delta \lambda)$ ,

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

$$\sigma_{\lambda}^{RSv} = \sigma_{\lambda}^{RSh} = 0, \tag{B.16}$$

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

<sup>652</sup> For perturbations in density  $(\delta \rho)$ ,

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

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

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

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

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

$$\overline{\sigma}_{\mu}^{RSv} = \frac{\omega^{3}k_{S}}{\pi c_{R}^{2} U_{R} \int (r_{1}^{2} + r_{2}^{2}) dz} \int \left[ \frac{1}{20} r_{1}^{2} + \frac{2}{15k_{R}^{2}} \left( \frac{\partial r_{2}}{\partial z} \right)^{2} - \frac{2}{15k_{R}} r_{1} \frac{\partial r_{2}}{\partial z} + \frac{7}{120} r_{2}^{2} + \frac{7}{120} r_{2}^{2} + \frac{7}{120k_{R}^{2}} \left( \frac{\partial r_{1}}{\partial z} \right)^{2} - \frac{7}{60k_{R}} \frac{\partial r_{1}}{\partial z} r_{2} \right] dz_{s} V^{2} \left( \frac{\delta \mu}{\mu_{0}} \right)^{2},$$
(B.21)

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

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### 654 B3 Rayleigh-to-Rayleigh-wave cross sections

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

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

$$\overline{\sigma}_{\mu}^{RR} = \frac{\omega^{3}\beta_{0}^{4}}{8c_{R}^{5}U_{R}^{2}[\int(r_{1}^{2}+r_{2}^{2})dz]^{2}} \int \left[3r_{1}^{4} + (r_{2} - \frac{1}{k_{R}}\frac{\partial r_{1}}{\partial z})^{4} + \frac{8}{k_{R}^{4}}\left(\frac{\partial r_{2}}{\partial z}\right)^{4} + \frac{8}{k_{R}^{2}}r_{1}^{2}\left(\frac{\partial r_{2}}{\partial z}\right)^{2}\right] dz_{s}V^{2}\left(\frac{\delta\mu}{\mu_{0}}\right)^{2}.$$
(B.25)

### 655 B4 Body-to-body-wave cross sections

<sup>656</sup> For perturbations in the Lamé parameter  $(\delta\lambda)$ ,

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

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

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

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

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

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

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

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

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

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

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

<sup>658</sup> and the averaged cross sections over incident angles

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

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

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

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

<sup>659</sup> For perturbations in shear modulus  $(\delta \mu)$ ,

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

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

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

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

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

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

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

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

660 and

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

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

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

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

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

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

#### 661 B5 Validation

We observe that

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

<sup>662</sup> The above relationship agrees with previous research about the cross-section ratios between P and S waves (Aki 1992). We can further write

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

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

We observe that the two body-wave expressions above, along with the expressions of  $\sigma^{PP}, \sigma^{SvP}, \sigma^{ShP}$  $\sigma^{ShP}$  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.

#### 667 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

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

for positive angular frequency  $\omega$ . In the last equality, the index n runs over all possible 674 eigenmodes of the elastodynamic operator  $L = -\alpha^2 \nabla \nabla \cdot + \beta^2 \nabla \times \nabla \times$  with eigenvalues  $\lambda_n$  and 675 displacement eigenfuction  $\phi_n$ . Notice that using  $\lambda$  to represent eigenvalues is custom in the 676 DOS theory and we only use this representation in this appendix. These eigenfunctions must 677 be normalized in the sense of the scalar product  $\langle \phi_n | \phi'_n \rangle = \int d^3 r \phi_n(\mathbf{x}) \phi'_n(\mathbf{x})^* = \delta_{n,n'}$ . In our 678 application, the index n will be continuous and all discrete sums become integrals as shown 679 below. The eigenfunctions of the operator L in an elastic halfspace bounded by a free surface 680 are plane Rayleigh wave and body-wave modes composed of an incident (normalized) plane 681 wave of a given polarization (P/Sv/Sh) together with its reflections. A rigorous diagonalization 682 of the operator L in a halfspace bounded by a free surface can be found in Sécher (1998) and 683

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:

$$N_{R} = 2\omega \int_{-\infty}^{+\infty} dk_{x} \int_{-\infty}^{+\infty} dk_{y} \frac{\delta(\omega^{2} - c_{r}^{2}(k_{x}^{2} + k_{y}^{2}))}{(2\pi)^{2}},$$
  
$$= \frac{\omega}{2\pi c_{R}^{2}}.$$
 (C.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:

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

which corresponds to the sum of an incident and a reflected plane wave with horizontal 696 unit polarization vector  $\mathbf{e}^{Sh}$  in the direction  $(k_y, -k_x, 0)$ . We take the vertical axis oriented 697 positively downward, so that a wavenumber -q < 0 (i.e. positive q) represents a up-going 698 wave. The eigenvalue associated to  $\phi_{Sh}$  is  $\lambda = \beta_0^2 (k_x^2 + k_y^2 + q^2)$  and the prefactor  $(2\pi)^{-3/2}$ 699 guarantees that the eigenfunction is correctly normalized. The squared modulus  $|\phi_{Sh}|^2$  is of 700 the form  $2 + 2\cos 2qz$  and presents oscillations (i.e.  $\cos 2qz$ ) due to the interference between 701 upgoing and downgoing waves. As these interferences are not taken into account in our model, 702 we average the DOS over depth to disentangle the upgoing and downgoing waves. Reporting 703 the result: 704

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

<sup>705</sup> into the DOS definition yields:

$$\langle N_{Sh} \rangle_z = 2\omega \int_0^{+\infty} dq \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{2\delta(\omega^2 - \beta_0^2(q^2 + k_x^2 + k_y^2))}{(2\pi)^3} \\ = \frac{\omega^2}{2\pi^2 \beta_0^3},$$
 (C.5)

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

<sup>707</sup> represent all possible incident (upgoing) plane Sh waves. The  $\delta$  function naturally selects only <sup>708</sup> those plane waves that satisfy the dispersion relation at frequency  $\omega$ .

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:

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

where  $\mathbf{e}^{P}$ ,  $\mathbf{e}^{P}_{r}$  and  $\mathbf{e}^{Sv}_{r}$  are unit polarization vectors in the directions  $(k_x, k_y, -q_p)$ ,  $(k_x, k_y, q_p)$ 712 and  $(-q_s, -q_s, k_x + k_y)$ , respectively. The first two polarizations are longitudinal and the 713 last one is transverse. The corresponding eigenvalue is  $\lambda = \alpha_0^2 (k_x^2 + k_y^2 + q_p^2)$ . The vertical S 714 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. 715 For the reflection coefficients, we use the standard notations from Aki & Richards (2002). 716 When we consider the quantity  $|\phi_p(\mathbf{x})|^2$ , cross terms involving P and S waves appear. Since 717 these terms are oscillatory, they cancel out when the squared eigenfunction is averaged over 718 depth, which in turn disentangles the P and S contributions: 719

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

<sup>720</sup> Eigenmodes for incident Sv waves have the form:

$$\phi_{Sv}(\mathbf{x}) = \frac{e^{i(k_x x + ik_y y)}}{(2\pi)^{3/2}} (e^{-iq_s z} \mathbf{e}^{Sv} + \acute{S} \grave{S} e^{iq_s z} \mathbf{e}_r^{Sv} + \acute{S} \grave{P} e^{iq_p z} \mathbf{e}_r^P)$$
(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

$$\langle |\phi_{Sv}(\mathbf{x})|^2 \rangle_z = \frac{(1+|\hat{S}\hat{S}|^2+|\hat{S}\hat{P}|^2)}{(2\pi)^3}.$$
 (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 730 yields:

$$\langle N_{Sv} \rangle_z = 2\omega \int_0^{+\infty} dq_s \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{\delta(\omega^2 - \beta_0^2 (q_s^2 + k_x^2 + k_y^2))}{(2\pi)^3} (1 + |\dot{S}\dot{S}|^2),$$

$$+ 2\omega \int_0^{+\infty} dq_p \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_y \frac{\delta(\omega^2 - \alpha_0^2 (q_p^2 + k_x^2 + k_y^2))}{(2\pi)^3} |\dot{P}\dot{S}|^2.$$
(C.10)

<sup>731</sup> Integrating over q and using polar coordinates for the horizontal wavenumbers integrals, we <sup>732</sup> get:

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

<sup>733</sup> We now make the substitution  $k \to \omega \sin j/\beta_0$ :

$$\langle N_{Sv} \rangle_z = \frac{\omega^2}{4\pi^2 \beta_0^3} \left( \int_0^{\pi/2} (1 + |\hat{S}\hat{S}|^2) \sin j dj + \int_0^{j_c} \frac{\beta_0 |\hat{P}\hat{S}|^2 \sin j \cos j dj}{\alpha_0 \cos i} \right),$$
(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:  $\beta_0 \cos j \hat{P} \hat{S} = \alpha_0 \cos i \hat{S} \hat{P}$ ; (2) Energy conservation:  $|\hat{S}\hat{S}|^2 + |\hat{S}\hat{P}|^2\alpha_0 \cos i/\beta_0 \cos j = 1$  for  $j \leq j_c$  and  $|\hat{S}\hat{S}|^2 = 1$  for  $j > j_c$ . Taking these elements into account, we arrive at the result:

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

<sup>738</sup> A similar treatment applied to P waves gives:

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

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  $\sigma^{RB}$  as the probability distribution of RB scattering at depth. We generate

<sup>751</sup> a possible depth for the scattered body wave (i.e. realizations of the distribution) using in-<sup>752</sup> verse transform sampling. This sampling method requires the cumulative distribution function <sup>753</sup> (CDF) of  $\sigma^{RB}$  and a random number (*rand*) uniformly distributed from 0 to 1. We then find <sup>754</sup> a depth ( $z_s$ ) which satisfies

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

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

$$CDF(z_s) = \frac{\int_0^{z_s} \sigma_{\rho}^{RSh} dz}{\int_0^{\infty} \sigma_{\rho}^{RSh} dz} = \frac{\int_0^{z_s} r_1^2(z,\omega) dz}{\int_0^{\infty} r_1^2(z,\omega) dz},$$
(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 757 (Figure D1). The main part of the PDF is distributed between the one Rayleigh-wave wave-758 length depth and the surface, and the CDF value is already close to 1 at the one wavelength 759 depth. Thus the scattering depth will be mostly distributed within one wavelength from the 760 surface. In practice, we do not compute the integral in the Monte Carlo simulations  $(\int_0^{z_s} \sigma^{RB} dz)$ 761 in Equation D.1), but instead calculate the CDF at some depths (zvec in Algorithm 4) prior 762 to the Monte Carlo simulation and then interpolate the depth (z) during the simulation (Al-763 gorithm 4). In the simulation, we choose the parameters about the depths as: Dz = 0.1 and 764 zmax = 10.765

# APPENDIX E: GENERATING SCATTERING AZIMUTHS AND COLATITUDES

We determine the type of scattered wave based on the cross sections of all possible scattered 768 waves, and we use the cross section of the scattered wave to determine the scattering azimuth 769 and colatitude. In calculating a cross section, we integrate the squared scattered-wave ampli-770 tudes along all possible scattering azimuths and colatitudes (e.g. Equation 8). A scattering 771 azimuth (colatitude) contributing more to the integral means that more scattered-wave energy 772 will be distributed at the azimuth (colatitude), which means the scattered wave will propagate 773 at the azimuth (colatitude) with a higher probability. Thus we interpret the integrand (e.g. in 774 Equation 8) as the PDF of scattering azimuth (colatitude). Following the same logic in Ap-775 pendix D, we use inverse transform sampling to generate scattering azimuths and colatitudes. 776 For example, in ShR scattering, we only need the scattering azimuth and then write the PDF 777

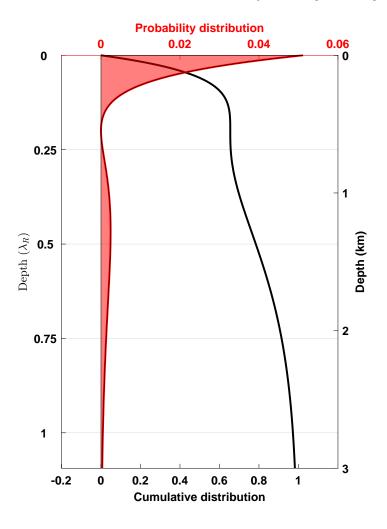


Figure D1. The probability and cumulative distributions of RSh scattering with depth.

778 of scattering azimuth as

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

<sup>779</sup> We observe that the scattering azimuth is more likely to be  $\pi/2$  and  $3\pi/2$  deg (90 and 270 <sup>780</sup> degree in Figure E1a), the azimuths orthogonal to the incident wave. No scattered Rayleigh <sup>781</sup> waves are expected at 0 or  $\pi$  (180 degree) for an incident Sh wave. These observations fit our <sup>782</sup> physical expectation in Section 2.2. We calculate the CDF based on Equation E.1, generate a <sup>783</sup> random number (*rand*) uniformly distributed from 0 to 1, and generate  $\xi_1$ , where  $CDF(\xi_1) =$ <sup>784</sup> *rand*. We use this same approach to generate random scattering azimuths for other scattering <sup>785</sup> (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 ( $\xi_1$ ) and colatitude ( $\psi_1$ ) is

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

<sup>795</sup> Notice that  $\psi_1$  and  $\xi_1$  are not required to be independent as in RP scattering. In such <sup>796</sup> a case, we need to generate a random azimuth and colatitude simultaneously. We write the <sup>797</sup> PDF for the two parameters in the RP scattering as:

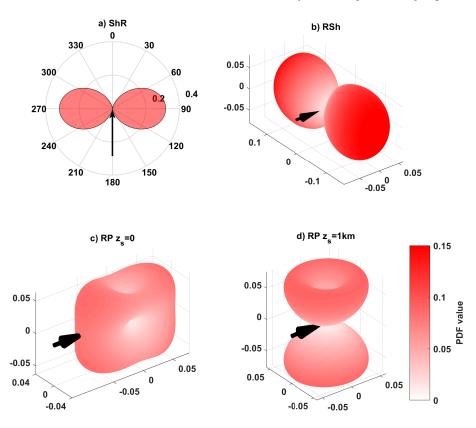
$$PDF(\xi_1, \psi_1, z_s) = \frac{\sum_m |A_{m,\rho}^{RP}|^2 \sin \psi_1}{\int_0^{\pi} \int_0^{2\pi} \sum_m |A_{m,\rho}^{RP}|^2 \sin \psi_1 d\xi_1 d\psi_1}$$
(E.3)  
$$= \frac{\left[r_1^2(z_s, \omega) \sin^2 \psi_1 \cos^2 \xi_1 + r_2^2(z_s, \omega) \cos^2 \psi_1\right] \sin \psi_1}{\int_0^{\pi} \int_0^{2\pi} \left[r_1^2(z_s, \omega) \sin^2 \psi_1 \cos^2 \xi_1 + r_2^2(z_s, \omega) \cos^2 \psi_1\right] \sin \psi_1 d\xi_1 d\psi_1}.$$
(E.4)

We observe that the distribution also depends on the scattering depth ( $z_s$ , Figure E1c and 798 E1d). In this case, we first determine  $z_s$  (Section D) and then find an azimuth and angle 799  $(\xi_{1,s} \text{ and } \psi_{1,s})$  which satisfy  $\int_0^{\xi_{1,s}} \int_0^{\psi_{1,s}} PDFd\xi_1 d\xi_1 = rand$  where rand is a random number 800 from a uniform distribution between 0 and 1. In practice, instead of calculating the integral 801  $(\int_0^{\xi_{1,s}} \int_0^{\psi_{1,s}} PDFd\xi_1 d\xi_1)$  in the simulations, we calculate a 2D CDF table for all possible  $\xi_{1,s}$ 802 and  $\psi_{1,s}$  prior to the simulation; for a more accurate table, we use the cosine values for 803 scattering colatitudes (i.e.  $\cos \psi_1$ ) instead of the colatitudes (Algorithm 5). Notice that due 804 to the cosine, we do not need to incorporate  $\sin \psi_1$  in the PDF function like the one in the 805 right end of the numerator of Equation E.4. 806

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

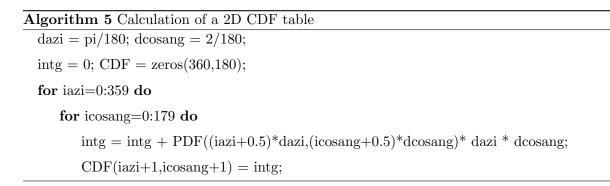
To illustrate how the free-surface boundary condition (FSBC) affects the simulation, we present the incident and reflected body-wave angular distributions on the free surface under

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**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 ( $\psi_1$ ) 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



between all the particle numbers and the P-wave particle number in the vertically up-going 818 bin, i.e.  $\cos(\psi_1) = -1$ . We average those ratios for the same wave type in a bin over a time 819 range such as first and last 50 Rayleigh-wave mean free times  $(\tau^R)$  in the simulation. We 820 refer to those averaged ratios with respect to  $\cos(\psi_1)$  as the angular distribution for each 821 type of wave on the free surface (Figure F1). We observe that, in the first 50  $\tau^R$ , where 822 the simulations are not yet in equipartition, the two FSBCs perform differently and lead 823 to two different body-wave angular distributions (Figure F1a and F1c). However, after the 824 simulations reach equipartition (Figure F1b and F1d), the incident and reflected body-wave 825 distributions for the two FSBCs are identical and symmetric along the zero cosine value (i.e. 826 parallel to the free surface). These symmetric body-wave angular distributions fit Lambert's 827 cosine law,  $|\cos(\psi_1)|$ , as in the diffusion theory. The  $(\alpha/\beta)^2$  for Sh/Sv waves is the intensity 828 ratio between P and Sv/Sh, because we actually calculate intensity based on the number of 829 particles encountering/leaving a surface, instead of energies based on the number of parti-830 cles in a space. Therefore we numerically demonstrate that the two FSBCs do not affect the 831 body-wave angular distribution on the free surface in the equipartition state. 832

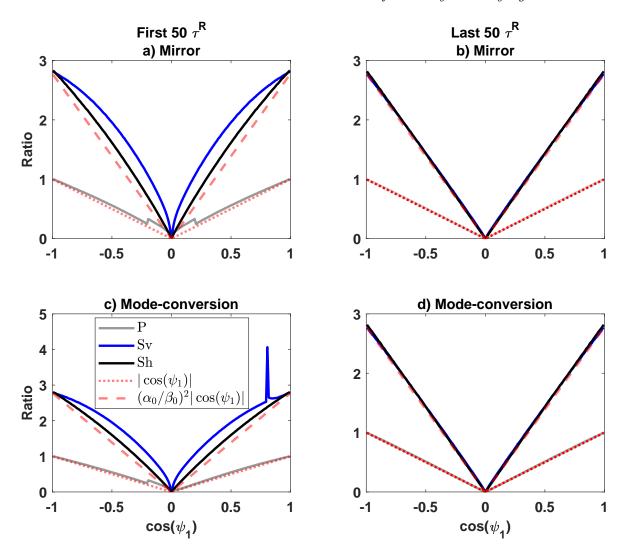


Figure F1. The body-wave angular distributions on the free surface under the mirror and modeconversion FBSCs in the first and last 50 Rayleigh-wave mean free times. The peak in c) is due to the P-Sv-wave coupling on the free surface.