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27 **Characterizing seismic scattering in 3D heterogeneous Earth by a single parameter**

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33

34 **Abstract**

35 We derive a theoretical parameter for three seismic scattering regimes where seismic  
36 wavelengths are either much shorter, similar, or much longer than the correlation length of small-scale  
37 Earth heterogeneities. We focus our analysis on the power spectral density of the von Karman  
38 autocorrelation function, used to characterize the spatial heterogeneity of small-scale variations of elastic  
39 rock parameters that cause elastic seismic wave scattering. Our theoretical findings are verified by  
40 numerical simulations. We discover 1) that seismic scattering is proportional to the standard deviation of  
41 velocity variations in all three regimes, 2) that scattering is inversely proportional to the correlation length  
42 for the regime where seismic wavelengths are shorter than correlation length, but directly proportional  
43 to the correlation length in the other two regimes, and 3) that scattering effects are weak due to  
44 heterogeneities characterized by a gentle decay of the von Karman autocorrelation function for regimes  
45 where seismic wavelengths are similar or much longer than the correlation length.

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47

48

## 49 Introduction

50 Heterogeneities in the Earth's crust and upper mantle cause seismic wave scattering, manifested  
51 in so-called seismic coda waves that trail the main seismic phases. Often, coda waves are prominent  
52 features of seismic recordings; they decay slowly with time, whereby the statistics of the temporal decay  
53 provide information about the scattering process and the medium through which the waves travelled (e.g.  
54 Aki 1969; Ritter et al., 1997; Sato and Fehler, 1998; Sato et al., 2012; Imperatori and Mai, 2013, 2015).  
55 After Aki's (1969) interpretation that coda waves are back-scattered energy from uniformly distributed  
56 heterogeneities in the Earth, several theoretical models were presented to explain seismic scattering, like  
57 the single scattering model, the multiple scattering model, the diffusion model, or the energy-flux model  
58 (Aki and Chouet, 1975; Sato, 1977; Gao et al., 1983; Frankel and Wennerberg, 1987). Additionally, the  
59 coda envelope broadens with increasing travel distance due to wavefield scattering (Sato 2016), a process  
60 that can be modelled employing a Markov approximation as stochastic treatment of the wave equation  
61 in random media (Sato et al., 2012; Sato 2016). In contrast, S-wave coda excitation is mainly dominated  
62 by scattering of direct S-waves from random heterogeneities in the Earth which can be modeled applying  
63 the Born approximation (Sato et al., 2012; Sato and Emoto, 2017). In summary, coda waves are seismic-  
64 wave energy trapped in the Earth due to the small-scale heterogeneities in the Earth.

65 Small-scale heterogeneities in the Earth can be described by a random spatial field superimposed  
66 onto a background homogeneous medium. For this purpose, several random-field models have been  
67 proposed; these are conveniently characterized by an autocorrelation function (ACF). For example, von  
68 Karman, Gaussian, exponential and Henyey–Greenstein ACF or a fractal distribution are used to describe  
69 random fields of seismic wave velocity variations in the Earth (e.g. Frankel and Clayton, 1986; Holliger and  
70 Levander, 1992; Sato and Fehler, 1998; Sato, 2019). Most commonly, the von Karman ACF is used (e.g.

71 Hartzell et al. 2010; Imperatori and Mai, 2013; Bydlon and Dunham, 2015). The power spectral density  
72 (PSD) of the von Karman AFC in three-dimension (3D) is given by

$$73 \quad p(k_m) = \frac{\sigma^2 (2\sqrt{\pi}a)^3 \Gamma(H + 1.5)}{\Gamma(H) (1 + k_m^2 a^2)^{(H+1.5)}}, \quad (1)$$

74 where  $a$ ,  $H$ ,  $\sigma$  and  $\Gamma$  are correlation length, Hurst exponent, standard deviation and the Gamma function,  
75 respectively. We denote the wavenumber ( $2\pi/\text{wavelength}$ ) of medium heterogeneity by  $k_m$ , and of the  
76 seismic wavefield by  $k_w$ , and write wavenumber  $k$  in case  $k_m$  and  $k_w$  can be used interchangeably.

77 Several studies examined the range for correlation lengths, standard deviation, and Hurst  
78 exponent in the Earth, both in observational studies and numerical simulations. Frankel and Clayton  
79 (1986) reported that velocity fluctuations with standard deviation of 5% and correlation lengths of 10 km  
80 (or greater) for 2D random media explain coda waves from micro earthquakes and travel time anomalies  
81 across seismic arrays. Holliger (1996) obtained correlation lengths of 10 to 100 meters and Hurst exponent  
82 in the range of 0.1 – 0.2 by analyzing sonic logs. Ritter et al. (1998) estimated wave-velocity perturbations  
83 of 3 – 7% and correlation length of 1 – 16 km for the lithosphere in central France. Recently, Sato (2019)  
84 reported that velocity perturbations are 1 – 10% in the Earth’s crust and upper mantle and that the Hurst  
85 exponent typically falls in the range 0.0 – 0.5, while correlation lengths vary widely depending on sample  
86 size or dimension of the measurement system. Overall, standard deviation, Hurst exponent, and  
87 correlation lengths are found to be in the range of 1 – 10%, 0.0 – 0.5, and 1 – 15 km, respectively.

88 Seismic wave scattering occurs as the elastic waves encounter spatial variations of elastic medium  
89 properties. Whilst even the deterministic reflection of a seismic wave at an internal interface of a seismic  
90 velocity contrast could be classified as “seismic scattering”, the common nomenclature is that seismic  
91 scattering is due to elastic-wave interactions with a spatially heterogeneous medium. In this context, the  
92 (statistical) characteristics of the scattered wavefield depend on the stochastic properties of the medium.

93 This concept is conveniently described considering the wavelengths ( $\lambda$ ) or wavenumbers ( $k_w$ ) of the elastic  
94 wave, and characteristic scales (wavelengths) of the random media.

95         Based on wavelength  $\lambda$  or wavenumber  $k_w$  of the seismic wave, and the correlation length  $a$  of  
96 the random media, seismic wave scattering can be classified into three regimes: (i)  $k_w a \gg 1$  ( $\lambda \ll a$ ); (ii)  
97  $k_w a \approx 1$  ( $\lambda \approx a$ ); (iii)  $k_w a \ll 1$  ( $\lambda \gg a$ ) (Sato and Fehler, 1998; Sato et al., 2012;). The regime  $k_w a \gg 1$   
98 characterizes high-frequency scattering in which seismic wavelengths are much shorter than correlation  
99 lengths. This regime is important for the earthquake engineering community in the context of high-  
100 frequency (10 – 20 Hz) ground-shaking estimation, because seismic scattering redistributes seismic wave  
101 energy (i.e. ground-motion amplitudes) in space and time. The regime  $k_w a \approx 1$  represents the diffraction  
102 condition, the most fundamental type of scattering. Finally, the regime  $k_w a \ll 1$  denotes low-frequency  
103 scattering for which seismic wavelengths are much longer than the correlation length of the random  
104 medium. This regime is important for global seismology which uses primarily long wavelengths (0.01 – 0.5  
105 Hz) to invert for the deterministic velocity structure of the Earth or earthquake source parameters (e.g.  
106 centroid moment tensors).

107         Numerical and theoretical studies investigating the effects of seismic scattering on earthquake  
108 ground-shaking suggest strong attenuation of ground-motion due to wavefield scattering (Shapiro and  
109 Kneib, 1993; Mai, 2009; Hartzell et al., 2010; Imperatori and Mai, 2012, 2013; Yoshimoto et al., 2015; Vyas  
110 et al., 2018). Bydlon and Dunham (2015) explained theoretically how the parameters describing the von  
111 Karman ACF control wavefield scattering in 2D. Using numerical simulations, they verified that a  
112 parameter  $\rho_0 = \sigma/a^H$  determines the nature of scattering in the  $k_w a \gg 1$  limit, regardless of the specific  
113 values of  $\sigma$  and  $a$ . However, how the other parameters of the von Karman ACF ( $a$ ,  $\sigma$  and  $H$ ) affect 3D  
114 seismic scattering has not been explored yet in detail.

115 Here, we investigate seismic wave scattering in 3D and verify our theoretical results by numerical  
116 simulations. First, we examine the mathematical expression for the power spectral density (PSD) of the  
117 von Karman AFC (Eq. 1) to identify parameters that represent scattering behaviour in 3D for the three  
118 different regimes,  $k_w a \gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$ . Then we test our theoretical findings through numerical  
119 simulations that cover the parameter space of these three regimes and allow us to examine how  
120 scattering manifests itself in seismic waveforms and ground-motion amplitudes.

121

## 122 Theory

123 Bydlon and Dunham (2015) investigated high-frequency scattering ( $f = 1 - 30$  Hz) by considering  
124 a 2D problem and the regime  $k_w a \gg 1$ . To analyze scattering under these assumptions, they simplified  
125 the PSD of the von Karman ACF to obtain the root-mean-square (RMS) fluctuations of normalized seismic  
126 wave velocity (wave speed), and then derived which parameters (i.e.,  $a$ ,  $H$  and/or  $\sigma$ ) control wavefield  
127 scattering. Here, we extend their approach to 3D by considering three different  $k_w a$  regimes.

128 Wavefield scattering is strongest if the wavenumber of the seismic wave is comparable to the  
129 wavenumber of heterogeneities in the medium. Hence, we simplify the PSD for the three regimes ( $k_w a$   
130  $\gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$ ) under the diffraction condition to obtain RMS of fluctuations of normalized  
131 wave velocity (computed as the square root of the mean power, denoted as  $P_{RM}$ ). By assuming the  
132 diffraction condition, we derive theoretically the parameter  $P_{RM}$ , which in fact dictates the wavefield  
133 scattering in 3D. Seismic scattering associated with a particular seismic wavelength will depend on the  
134 amplitudes of velocity variations corresponding to that wavelength. However, we aim to understand the  
135 overall wavefield scattering behaviour for a range of seismic wavelengths and heterogeneity scales in the  
136 medium. Therefore, our  $P_{RM}$  derivations are not only applicable for a monochromatic source or a single-  
137 wavelength medium, but instead capture the broadband nature of scattering. Note that we only

138 summarize the final equations for  $P_{RM}$  for each regime in the main text; further details of the derivations  
 139 are provide in the Electronic supplement.

140

141 **Regime I:  $k_w a \gg 1$**

142 Our  $P_{RM}$  derivation for this regime assumes that the source excites waves of equal amplitude (a  
 143 flat source spectrum) with wavenumbers from  $k_{min}$  to infinity, all of which interact with heterogeneities in  
 144 the medium with the same range of wavenumbers (albeit at different “intensity” or strength). Note that  
 145 this assumption is not completely satisfied in nature as earthquakes typically excite only a limited range  
 146 of frequencies, and not all of these frequencies will interact with the generally scale-limited medium  
 147 heterogeneities. However, the assumption allows us to calculate the overall wavefield scattering  
 148 behaviour for the regime  $k_w a \gg 1$ , for which seismic wavelengths are much shorter than the correlation  
 149 length of small-scale Earth heterogeneities. Then, the RMS fluctuations of normalized wave velocity ( $P_{RM}$ )  
 150 can be approximated by

$$151 \quad P_{RM} = \sqrt{\frac{1}{4\pi} \int_{k_{min}}^{\infty} p(k) k^2 dk} \approx \sqrt{(c_0 + c_1 H + c_2 H^2)} \frac{\sigma}{a^H} \frac{\pi^{1/4}}{k_{min}^H} \quad (2)$$

152 Therefore, the  $P_{RM}$  dependency is given by,

$$153 \quad P_{RM} \propto \sqrt{(c_0 + c_1 H + c_2 H^2)} \frac{\sigma}{a^H}, \quad (3)$$

154 where we approximate the term depending on  $H$  by a quadratic function (with coefficients  $c_0= 0.89$ ,  $c_1=$   
 155  $0.53$ , and  $c_2= -0.08$ ; see Fig. S1a and derivation in electronic supplement for details). Note that we  
 156 characterize the scattering behavior for the entire regime  $k_w a \gg 1$ , rather than for a particular wavelength  
 157 in this regime by using integration limits in Eq. 2 from  $k_{min}$  to infinity, and not over any arbitrary  
 158 wavenumber range. Therefore, the parameter  $P_{RM}$  (Eq. 3) becomes independent of wavenumber.

159 Comparing Eq. 3 with parameter  $p_0 = \sigma/a^H$  (Bydlon and Dunham, 2015) reveals that even in the regime  
 160  $k_w a \gg 1$ , scattering in 3D is more complex than in 2D. Eq. 3 illustrates that in the high-frequency scattering  
 161 regime, (a) scattering is proportional to the standard deviation of the velocity fluctuations, (b) scattering  
 162 is inversely proportional to the correlation length  $a$ , and c) the Hurst exponent has a strongly non-linear  
 163 effect on scattering. Interestingly, if the Hurst exponent approaches its theoretical lower limit of zero  
 164 ( $H \rightarrow 0$ ), Eq. 3 can be further simplified to

$$165 \quad P_{RM} \propto \sigma, \quad (4)$$

166 indicating that scattering is controlled by the standard deviation of the velocity variations in this case.

167

168 **Regime II:  $k_w a \approx 1$**

169 We assume that the source excites waves having a flat source spectrum with wavenumbers from  
 170  $k_1$  to  $k_2$ , all of which interact with medium heterogeneities of the same wavenumber range. If seismic  
 171 wavelengths are comparable to the correlation length of heterogeneities, the RMS fluctuations of  
 172 normalized wave velocity can be approximated by

$$173 \quad P_{RM} = \sqrt{\frac{1}{4\pi} \int_{k_1}^{k_2} p(k) k^2 dk} \approx \left(\frac{\pi}{18}\right)^{1/4} a^{3/2} \sigma \sqrt{(c_1 H + c_2 H^2)} \sqrt{(k_2^3 - k_1^3)} \quad (5)$$

174 Therefore, the  $P_{RM}$  dependency is given by,

$$175 \quad P_{RM} \propto \sqrt{(c_1 H + c_2 H^2)} a^{3/2} \sigma, \quad (6)$$

176 Where coefficients are given as  $c_1 = 0.93$ , and  $c_2 = -0.27$  (see Fig. S1b). Analyzing Eq.6 for  $P_{RM}$  reveals that  
 177 a) scattering is proportional to  $\sigma$ , similar to the regime  $k_w a \gg 1$ , b) scattering is proportional to correlation  
 178 length  $a$ , in contrast to regime  $k_w a \gg 1$  (compare Eq. 6 with Eq. 3), and c) scattering is correlated with the  
 179 Hurst exponent (as  $H$  approaches zero, scattering effects weaken and become eventually negligible).

180

181 **Regime III:  $k_w a \ll 1$**

182 Here, we assume that the source excites waves of equal amplitude (a flat source spectrum) with  
183 wavenumbers from zero to  $k_1$ , all of which interact with medium heterogeneities. If seismic wavelengths  
184 are much longer than the correlation length of the heterogeneities, the RMS fluctuations of normalized  
185 wave velocity can be approximated by

186 
$$P_{RM} = \sqrt{\frac{1}{4\pi} \int_0^{k_1} p(k) k^2 dk} \approx \left(\frac{4\pi}{9}\right)^{1/4} a^{3/2} \sigma \sqrt{(c_1 H + c_2 H^2)} k_1^{3/2} \quad (7)$$

187 Therefore, the  $P_{RM}$  dependency is given by

188 
$$P_{RM} \propto \sqrt{(c_1 H + c_2 H^2)} a^{3/2} \sigma, \quad (8)$$

189 where coefficients  $c_1 = 0.93$ , and  $c_2 = 0.40$  (see Fig. S1c). Note that only constant  $c_2$  is different between  
190 Eq. 8 and Eq. 6, therefore,  $P_{RM}$  for the regime  $k_w a \ll 1$  is similar to that for  $k_w a \approx 1$ , except that the effect  
191 of  $H$  on scattering is stronger for  $k_w a \ll 1$  than for  $k_w a \approx 1$  because  $c_2 > 0$  (compare Eq. 6 and Eq. 8).

192

193 **Verification of Theory by Simulations**

194 In this section, we verify our findings (Eq. 3, 4, 6, 8) by conducting seismic wavefield simulations  
195 in random media. Since our simulations do not strictly satisfy the assumptions used for the derivations of  
196  $P_{RM}$ , we validate only proportionality or inverse-proportionality of  $P_{RM}$  with correlation length, standard  
197 deviation, and Hurst exponent, rather than the complete expressions (Eq. 3, 4, 6, 8). To numerically test  
198 our results for the three scattering regimes, we fix the correlation length  $a$  and modify the source  
199 frequency to radiate seismic waves with different frequencies (i.e., we are altering the wavenumber  $k_w$ ).  
200 For computing synthetic seismograms, we use a generalized 3D finite-difference method with second-

201 order accuracy in space and time (SORD code by Ely et al., 2008). Our simulations consider several  
202 discretized Earth models, a point-source earthquake model, and receiver locations at which ground-  
203 motions are stored. We then analyze waveforms and peak ground acceleration (PGA), and confront the  
204 numerical results with our theoretical analysis.

205

### 206 ***Set up for Numerical Modeling***

207 We consider a point source (moment magnitude  $M_w \sim 2.84$ ) at a depth of 7.5 km, with strike, dip,  
208 and rake of  $22.5^\circ$ ,  $90^\circ$ , and  $0^\circ$ , respectively. The source-time function (STF) is a Gaussian. We define STFs  
209 to radiate frequencies required to properly sample the three regimes ( $f_{max} = 5.0$  Hz for  $k_w \cdot a \gg 1$ ,  $f_{max} = 0.5$   
210 Hz for  $k_w \cdot a \approx 1$  and  $f_{max} = 0.03$  Hz for  $k_w \cdot a \ll 1$ , see Fig S2;  $f_{max}$  is the high frequency limit of the flat portion  
211 of the slip velocity spectrum). For example, a point source radiating frequencies of 5.0 Hz, 0.5 Hz and 0.03  
212 Hz in a heterogeneous medium with background shear-wave velocity 3.464 km/s and stochastic  
213 perturbations with correlation length of 1 km yields  $k_w \cdot a \approx 9.0$ , 0.9 and 0.05, respectively.

214 To create a velocity model with small-scale heterogeneities, we add random-field variations of  
215 seismic wave velocities, characterized by an isotropic von Karman ACF, to the uniform background Earth  
216 model (with S-wave velocity 3464 m/s, P-wave velocity, 6000 m/s, and density  $2700 \text{ kg/m}^3$ ). In total, we  
217 generate twelve 3D computational models (M1 to M12; Table 1), considering three correlation lengths  
218 (1.0 km, 5.0 km, 10.0 km), two values of standard deviation (5%, 10%), and two Hurst exponents (0.1, 0.5).  
219 For each combination of medium parameters, we create one realization of random inhomogeneity in S-  
220 wave speed, P-wave speed, and density. S-wave velocity distributions at the surface are shown for all  
221 twelve computational models (Figs 1a, 1b). Theoretical 1D power spectra for seven selected models are  
222 plotted to illustrate effects of correlation lengths, standard deviation, and Hurst exponent on the spectral

223 shape (Fig 1c). Power spectra for two specific models, M2 and M11, are examined for the three scattering  
224 regimes considering the three STFs used in this study (Fig. 1d).

225           The size of the computational domain must be chosen such that seismic waves propagate to large-  
226 enough distances that ensure sufficient wave interaction with medium heterogeneities to develop  
227 scattering. At the same time, the domain should be as small as possible to minimize computational cost.  
228 Given these constraints, we define different computational domain sizes and grid spacings, depending on  
229 scattering regime. For the regime  $k_w a \gg 1$ , we use grid spacing  $h=25\text{m}$  ( $dt=0.0015\text{ s}$ ) on a domain of  
230  $60 \times 60 \times 15\text{ km}$ , allowing travel distance of  $\sim 40$  wavelengths (at  $f = 5.0\text{ Hz}$ ). Combining these models with  
231 STF1 (Fig. S2a) yields  $k_w a$  in the range of 9 to 90. For  $k_w a \approx 1$  we use  $h=75\text{m}$  ( $dt=0.0045\text{ s}$ ) and a larger  
232 domain,  $355 \times 355 \times 30\text{ km}$ , corresponding to travel distance of  $\sim 50$  wavelengths (at  $f = 0.5\text{ Hz}$ ). The eight  
233 corresponding models are denoted by the suffix “-L” (see Tab 1 and Fig S3) and when combined with STF2  
234 (Fig. S2b), they result in  $k_w a$  -values between 0.9 and 4.5. For  $k_w a \ll 1$ , we use  $h=1000\text{m}$  ( $dt=0.055\text{ s}$ ) and  
235 an extra-large domain,  $2000 \times 2000 \times 60\text{ km}$  (ignoring the spherical nature of Earth), denoted by the suffix  
236 “-EL” (see Tab 1 and Fig S4). When combined with STF3 (Fig. S2c), the corresponding  $k_w a$  values fall in the  
237 range 0.27 to 0.5. Owing to the very long wavelengths in this regime ( $\sim 115\text{km}$  at  $f = 0.03\text{ Hz}$ ), the domain  
238 allows travel distances of only  $\sim 15$  wavelengths, significantly lower than those in the two previous  
239 regimes. However, the cost for computational models allowing travel distances of  $\sim 45\text{-}50$  wavelengths  
240 would be exorbitant. In total, we use 28 computational models with random inhomogeneities, twelve of  
241 which are for  $k_w a \gg 1$ , eight for  $k_w a \approx 1$  and eight for  $k_w a \ll 1$  regimes. Our simulations consumed nearly  
242 four million core-hours of computational resources on a Cray XC40 supercomputer. To establish a base  
243 case for comparison, we also conduct simulations in a homogeneous medium for each regime.

244           We store synthetic seismograms at receivers placed in a concentric rings for  $k_w a \gg 1$ , but for  $k_w a$   
245  $\approx 1$  and  $k_w a \ll 1$  we consider only a one quadrant to save computational costs (Fig 1a, Fig S3a, Fig S4a).  
246 The epicenter is placed in the center of the simulation domain for  $k_w a \gg 1$ , but for  $k_w a \approx 1$  and  $k_w a \ll 1$

247 it is in the lower left corner. Receiver geometry and epicenter location are designed to obtain the best  
248 possible azimuthal coverage of stations and to allow for sufficiently large travel distances for seismic  
249 waves to develop scattering, at the same time also minimizing computational costs. Virtual stations are  
250 distributed along rings with radial spacing of 0.1, 0.2 and 3.5 km, for  $k_w a \gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$   
251 regimes, respectively. Therefore, each ring (arc) of stations contains a different number of stations at  
252 different azimuths. The smallest ring (arc) used for PGA statistics has 314 (radius 5km), 196 (radius 25 km)  
253 and 134 (radius 300 km) stations for the three regimes ( $k_w a \gg 1$ ;  $k_w a \approx 1$ ;  $k_w a \ll 1$ ). Therefore, our  
254 receiver geometry is statistically independent and PGA statistics are robust. All waveforms are low-pass  
255 filtered using a fourth-order Butterworth filter with cutoff frequencies of 5 Hz, 0.5 Hz and 0.03 Hz for the  
256 three scattering regimes, respectively.

257

### 258 ***Quantifying Seismic Scattering in Numerical Results***

259 Seismic scattering redistributes energy in space and time from direct P- and S-waves into the late-  
260 arriving coda waves. Consequently, peak ground acceleration (PGA) in a homogeneous medium will be,  
261 on average, higher than in a scattering medium. Therefore, we examine ratios of PGA-values to quantify  
262 scattering “strength” in numerical simulations. Horizontal components of acceleration are mostly used in  
263 earthquake engineering applications (e.g., Boore and Atkinson, 2008; Chiou and Youngs, 2008), because  
264 wave amplitudes on the vertical component are usually smaller than on the horizontal components.  
265 Therefore, we analyze horizontal PGA (computed as maximum magnitude of acceleration from the two  
266 horizontal components). We illustrate scattering effects and resulting PGA values by comparing  
267 waveforms for selected receivers s1, s2 and s3 (see Fig 1a for their locations).

268 In Fig 2 we compare horizontal-component ground-acceleration waveforms at selected stations  
269 for the regime  $k_w a \gg 1$ . Fig 2a compares waveforms and PGA values for two values of standard deviation

270 (models M3 and M6) with those for the homogeneous medium PGA values are consistent with our  
271 expectation that stronger scattering leads to lower PGA. In this particular case, the scattering for model  
272 M3 is weaker than for model M6 (see also acceleration snapshots in Fig S5). Additionally, ground  
273 acceleration comparison for M6 at three stations (Fig S6) shows prominent coda evolution and reduced  
274 maximum acceleration values as epicentral distance increases (from  $s_4$  to  $s_6$ ). Fig 2b reveals that  
275 waveforms for two models with different correlation lengths (M1 and M3) are almost identical, with only  
276 small time shifts. This indicates that the two models yield almost identical levels of scattering (confirmed  
277 also by comparing acceleration snapshots for M1 and M3 in Fig S5). Correspondingly, PGA values are  
278 comparable. In addition, these comparisons (Figs 2a and 2b) suggest that scattering is primarily controlled  
279 by the standard deviation of the medium heterogeneities, whereas the correlation length has a negligible  
280 effect for a small  $H$  value ( $H = 0.1$ ), consistent with our theoretical analysis in Eq. 4. However, we note that  
281 PGA only works well in such comparisons because we computed a reference solution for the  
282 homogeneous medium. Without such a reference case, interpreting PGA values directly as indicator for  
283 “scattering strength” would be misleading.

284

### 285 ***Statistical Analysis of Scattering***

286         Next, we calculate the mean and standard deviation of PGA values for all stations at a given  
287 epicentral distance and for a given computational model (see Fig. S7 for a comparative summary of all  
288 computational models). To estimate the average scattering-related PGA reduction at a given epicentral  
289 distance, we define the “mean PGA ratio” (MPR), at a particular epicentral distance, as the ratio between  
290 the mean PGA values from any heterogeneous Earth model to the mean PGA-values from the reference  
291 homogeneous Earth model. As epicentral distance increases, the MPR is expected to decrease because  
292 the redistribution of seismic energy due to scattering is cumulative with propagation distance.

293 Figure 3 summarizes our results for  $k_w a \gg 1$ . For  $H = 0.1$  we find the MPRs for models with  $\sigma =$   
 294 10% (M4, M5, M6) are lower than for models with  $\sigma = 5\%$  (M1, M2, M3) (Fig. 3a). At the same time, MPRs  
 295 of both groups are very similar, supporting our theoretical conclusion that for small  $H$  the correlation  
 296 length has insignificant effects on scattering, which in this regime is controlled by standard deviation (Eq.  
 297 4). The apparent plateau in MPRs for distances 10 to 20 km is a consequence of source effects being  
 298 masked by wavefield scattering effects due to the hypocenter location (see Fig. S8 for more details on the  
 299 effects of hypocentral depths on MPRs). Fig 3b compares solutions for  $H=0.5$ , for which we expect a  
 300 significant effect of both correlation length and standard deviation. For fixed  $\sigma$ , we observe that the MPR's  
 301 for models with shorter correlation length are lower than those with longer correlation length ( $MPR_{M7} <$   
 302  $MPR_{M8} < MPR_{M9}$ ; similarly  $MPR_{M10} < MPR_{M11} < MPR_{M12}$ ). This finding is consistent with our conclusion  
 303 that scattering is inversely proportional to correlation length for large  $H$  (Eq. 3). Also, MPR's for models  
 304 with  $\sigma = 10\%$  are lower than those for corresponding models with  $\sigma = 5\%$  ( $MPR_{M10} < MPR_{M7}$ ,  $MPR_{M11} <$   
 305  $MPR_{M8}$ ,  $MPR_{M12} < MPR_{M9}$ ), demonstrating that scattering is proportional to the standard deviation of  
 306 velocity variations for large  $H$ . Thus, these observations validate our theoretical conclusions for the regime  
 307  $k_w a \gg 1$ .

308 The MPR-analysis for regime  $k_w a \approx 1$  is summarized in Figure 4. For both values of  $H$ , the MPR's  
 309 for models with shorter correlation length are higher than MPR's for models with longer correlation length  
 310 ( $MPR_{M1-L} > MPR_{M2-L}$ ,  $MPR_{M4-L} > MPR_{M5-L}$ ,  $MPR_{M7-L} > MPR_{M8-L}$ ,  $MPR_{M10-L} > MPR_{M11-L}$ ),  
 311 revealing that scattering is proportional to correlation length (see Fig. 4a and Fig. 4b). The MPR's for  
 312 models with  $\sigma = 5\%$  are higher than those for model with  $\sigma = 10\%$  ( $MPR_{M1-L} > MPR_{M4-L}$ ,  $MPR_{M2-L} >$   
 313  $MPR_{M5-L}$ ,  $MPR_{M7-L} > MPR_{M10-L}$ ,  $MPR_{M8-L} > MPR_{M11-L}$ ), indicating that scattering is proportional to  
 314 the standard deviation of velocity fluctuations. The MPR's for models with  $H = 0.1$  are larger than those  
 315 for models with  $H = 0.5$  ( $MPR_{M1-L} > MPR_{M7-L}$ ,  $MPR_{M2-L} > MPR_{M8-L}$ ,  $MPR_{M4-L} > MPR_{M10-L}$ ,

316  $MPR_{M5-L} > MPR_{M11-L}$ ), therefore, scattering is proportional to the Hurst exponent  $H$ . These  
317 observations are also consistent with our theoretical findings for  $k_w a \approx 1$  (see Eq. 6).

318 Finally, we show MPR statistics for the regime  $k_w a \ll 1$  (Figure 5). First, recall that due to  
319 prohibitively large computational costs we used a smaller computational domain (see Section *Set up for*  
320 *Numerical Modeling*). Consequently, scattering is less well developed for  $k_w a \ll 1$ , and hence effects on  
321 MPR's are not as pronounced as in the other two regimes. Still, the effects are strong enough to support  
322 our theoretical derivation (see waveform comparison in Fig. S9 and station locations in Fig. S4). The MPR's  
323 for models with 10 km correlation length are lower than those for 5 km correlation length ( $MPR_{M3-EL} <$   
324  $MPR_{M2-EL}$ ,  $MPR_{M6-EL} < MPR_{M5-EL}$ ,  $MPR_{M9-EL} < MPR_{M8-EL}$ ,  $MPR_{M12-EL} < MPR_{M11-EL}$ ), showing  
325 that scattering is proportional to correlation length. The MPR's for models with  $\sigma = 10\%$  are lower than  
326 those for  $\sigma = 5\%$  ( $MPR_{M12-EL} < MPR_{M9-EL}$ ,  $MPR_{M11-EL} < MPR_{M8-EL}$ ), suggesting that scattering is also  
327 proportional to the standard deviation of velocity variations. These observations agree well with our  
328 theoretical considerations for  $k_w a \ll 1$  (see Eq. 8).

329 In summary, our results from numerical simulations are consistent with our conclusions based on  
330 theoretical derivation for all three considered scattering regimes.

331

## 332 Discussion and Conclusions

333 We derive a new parameter  $P_{RM}$  to quantify 3D seismic wavefield scattering.  $P_{RM}$  is based on the  
334 assumption that small-scale heterogeneities in seismic velocity are characterized by the von Karman ACF.  
335  $P_{RM}$  helps to understand the influence of the parameters of the von Karman ACF on seismic scattering for  
336 three considered regimes ( $k_w a \gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$ ). We test our theoretical consideration through

337 statistical analysis of a suite of numerical simulations that capture seismic scattering in different scattering  
338 regimes.

339 We find that the strength of wavefield scattering in all three regimes is proportional to the  
340 standard deviation of heterogeneities. Seismic scattering is also proportional to the correlation length in  
341 the regimes  $k_w a \approx 1$  and  $k_w a \ll 1$ , but for the regime  $k_w a \gg 1$  the scattering is inversely proportional to  
342 correlation length. For regime  $k_w a \gg 1$ , we also find that if the Hurst exponent  $H$  approaches zero,  
343 scattering will be controlled solely by standard deviation. However, for  $k_w a \approx 1$  and  $k_w a \ll 1$ , scattering  
344 is weakly impacted for small values of  $H$ , with scattering vanishing in the limit of  $H \rightarrow 0$ .

345 To further explain these findings, we integrate the PSD for the 3D problem (Eq. 1) with respect to  
346 wavenumber  $k_m$ ,

$$347 \int_0^{\infty} p(k_m) dk_m = 4\pi^2 a^2 \sigma^2 H \quad (9)$$

348 Eq. 9 represents the area under the power spectrum for a three dimensional isotropic PSD along one  
349 wavenumber axis; it reveals that the area under the power spectrum depends on  $a$ ,  $H$  and  $\sigma$ , implying also  
350 that the area under the power spectrum will be zero if any of  $a$  or  $H$  or  $\sigma$  is zero. For example, M2 has  
351 larger area under the power spectrum than M1 due to larger correlation lengths of M2, although standard  
352 deviation and Hurst exponent are identical for M1 and M2 (see Fig. 1c). The area under the power  
353 spectrum can be linked to wavefield scattering as it represents the total scattering power of the  
354 heterogeneous medium in terms of the sum of amplitude squares of seismic-velocities. Correspondingly,  
355 in the limit of any of the von Karman parameters approaching zero, wavefield scattering will become  
356 negligible.

357 Quantitative analysis of power spectra in Fig 1c helps to interpret the implications of Eq. 9 for the  
358 three scattering regimes. Therefore, our theoretical findings, confirmed by numerical simulations, can be

359 explained by the amplitude and shape of the PSD. The standard deviation scales the power spectra  
360 without changing the shape of the power spectra (hence, area under the power spectra), resulting in  
361 scattering proportional to  $\sigma$  for all three regimes ( $k_w a \gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$ ). The tails of the power  
362 spectra (decaying part) show inverse proportionality with correlation length  $a$  (e.g. compare tails of M7,  
363 M8 and M9 in Fig 1c), thus resulting in scattering being inversely proportional to  $a$  for the regime  $k_w a \gg$   
364  $1$ . However, the plateau and corners (corner wavenumber =  $2\pi/a$ ) of the power spectra scale with  
365 correlation length, leading to scattering being proportional to correlation length for  $k_w a \ll 1$  and  $k_w a \approx$   
366  $1$ , respectively (e.g. compare plateau and corners of M7, M8 and M9 in Fig 1c). Furthermore, the plateau  
367 and corner of power spectra grow as  $H$  increases, therefore, scattering is proportional to  $H$  for  $k_w a \ll 1$   
368 and  $k_w a \approx 1$ . Fig 1c also shows that the tails of the power spectra tend to merge for small  $H$  (see M1, M2  
369 and M3) and diverge as  $H$  increases (compare M7, M8 and M9), implying a more complex dependency on  
370  $H$  for scattering in the regime  $k_w a \gg 1$ . Hence, our findings can be explained by the shape and amplitude  
371 of the PSD function of the von Karman ACF.

372 Comparing our results for  $k_w a \gg 1$  for the 3D problem (Eq. 3) with the 2D results by Bydlon and  
373 Dunham (2015) ( $p_0 = \sigma/a^H$ ) reveals that the effect of standard deviation and correlation length remains  
374 the same, but the effect of the Hurst exponent  $H$  is stronger in 3D. However, if the Hurst exponent  
375 approaches zero, scattering effects are dominated by standard deviation, both in 2D and 3D. This is an  
376 important finding, since values of  $H$  smaller than 0.5 have been reported by Sato (2019) for the Earth's  
377 crust and mantle.

378 Here we propose to quantify the overall wavefield scattering directly via an integral of the PSD  
379 function of the random media. We note that Sato et al. (2012) analyzed a plane wave scattered by a  
380 localized inhomogeneity using the wave equation. They solved the wave equation utilizing Born  
381 approximation, i.e., they assumed that the amplitude of velocity variations is negligibly small compared

382 to background velocity, that the amplitude of the scattered wavefield is negligibly small compared to the  
 383 amplitude of incident wavefield, and that the scattered wavefield has only a small phase change after  
 384 passing through the heterogeneity. Therefore, derivations by Sato et al., (2012) are valid for high  
 385 frequency scattering, when seismic wavelengths are very short compared to the length scales of medium  
 386 heterogeneity. They found that the scattering coefficient depends on the PSD function of the random  
 387 media as follows (Eq. 4.25 from Sato et al., 2012),

$$388 \quad g(\theta, \omega) = \frac{k_w^4}{\pi} P(2k_w \sin \frac{\theta}{2}) \quad (10)$$

389 In Eq. 10,  $\theta$  is the angle between incident and scattered waves;  $\omega$  and  $k_w$  are angular frequency  
 390 and wavenumber of the incident wavefield, respectively. The scattering coefficient reveals that a wave  
 391 with wavenumber  $k_w$  interacts with medium heterogeneities with wavenumber  $k_m$ , leading to

$$392 \quad k_m = 2k_w \sin \frac{\theta}{2} = 2 \sin \frac{\theta}{2} k_w = C k_w \quad (11)$$

393 The scaling factor  $C$  is a function of the scattering angle  $\theta$  and ranges from 0 to 2, for forward ( $\theta$   
 394 = 0) and backward ( $\theta = \pi$ ) scattering, respectively. The average value of  $C$  (over  $\theta$ ) indicates the overall  
 395 interaction between  $k_m$  and  $k_w$ , averaged over all directions. The average value of  $C$  is 1.27, therefore  $k_m$   
 396  $\sim k_w$ . This is consistent with our assumption for the derivation of  $P_{RM}$ , although we apply an ideal  
 397 diffraction condition ( $k_m = k_w$ ). Note that our  $P_{RM}$  results will not change even if we use a more relaxed  
 398 diffraction condition (i.e.  $k_m \sim k_w$ ). Hence, our theory complies with Sato et al. (2012), but taking a different  
 399 perspective on evaluating the wavefield scattering. Note that the detailed theoretical analysis to fully  
 400 describe the wavefield scattering in 3D requires considering the 3D elastic wave equation with complex  
 401 earthquake source characteristics (radiated wavefield) in 3D random media with anisotropic wave  
 402 propagation. This derivation is beyond the scope of the present study.

403           In summary, our theoretical analysis of the von Karman PSD, used to represent random spatial  
404 variation in seismic wave velocities and rock density, helps to develop a physics-based understanding of  
405 how standard deviation, correlation length, and Hurst exponent govern three-dimensional seismic  
406 wavefield scattering for three scattering regimes ( $k_w a \gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$ ). This will help studies  
407 on ground-motion simulations for earthquake shaking as well as research on global seismic wave  
408 propagation in 3D Earth models to properly simulate elastic wavefield scattering.

409

## 410 **Data and Resources**

411           Ground-motions simulations carried out to verify the outcomes of theoretical derivation  
412 generated nearly 2.5 TB of data which can be provided via personal communication. This manuscript has  
413 an electronic supplement which comprises the complete derivation of the root-mean-square fluctuations  
414 of normalized wave velocity using power spectral density of the von Karman autocorrelation function for  
415 three scattering regimes ( $k_w a \gg 1$ ,  $k_w a \approx 1$  and  $k_w a \ll 1$ ). The electronic supplement also contains figures  
416 of the quadratic fit to ratios of gamma functions, three Gaussian source time functions, simulations setup  
417 depicting receiver geometry and S-wave speed variations, acceleration waveforms comparison from few  
418 receivers, snapshots of ground-acceleration wavefield at Earth surface and peak ground acceleration  
419 statistics.

420

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538 **List of Table Captions**

539 **Table 1:** Parameters for the 28 computational 3D Earth models generated for this study.

540

541 **List of Figure Captions**

542 **Figure 1: (a,b):** S-wave speed distribution at the free surface for twelve 3D computational models for the  
543 regime  $k_w a \gg 1$ , generated using three correlation lengths (1.0 km, 5.0 km, 10.0 km), two standard  
544 deviations (5%, 10%) and two Hurst exponents (0.1, 0.5). The black star marks the epicenter. The sites  
545 used for waveform comparison (black triangles, s1, s2, s3, s4, s5 and s6) and ground-motion analysis (black  
546 dots in circular rings) are also shown. The beach ball shows the focal mechanism of the earthquake source.  
547 Panels (a) and (b) depict random media with Hurst exponent 0.1 and 0.5, respectively. **(c):** Theoretical 1-  
548 D power spectra (PSD) for 3D Earth structure for seven selected models. Correlation length and Hurst  
549 exponent alter the shape of the power spectra (solid lines), whereas standard deviation only scales the  
550 PSD (mark dashed line; notice the scaling of M4 compared to M1, but their identical shape). **(d):** The  
551 theoretical power spectra of the random media are constrained by the dimensions of the computational  
552 model and the spatial grid size. The dashed and solid lines are spectra related to models M2 and M11,  
553 whereas three different colors depict power spectra sampled according to the three scattering regimes.

554

555 **Figure 2:** Horizontal components (East-West, EW, and North-South, NS) of ground acceleration ( $m/s^2$ ) at  
556 sites s1, s2, s3 (Fig 1a). Black dotted lines indicate theoretical P- and S-wave arrival times in the considered  
557 homogeneous medium. Color-coded numbers indicate PGA values at individual sites. Waveforms are  
558 normalized by their PGA-value in the homogeneous-medium simulations for a given site. (a) Illustration

559 of scattering controlled by  $\sigma$  for  $k_w a \gg 1$  and small  $H$ ; (b) Illustration of negligible effects of correlation  
560 length on scattering for  $k_w a \gg 1$  and small  $H$ .

561

562 **Figure 3:** Mean PGA ratios (MPR) for all twelve numerical simulations as a function of distance, depicting  
563 the effects of wavefield scattering on ground-motions in the regime  $k_w a \gg 1$ . Panels (a) and (b) depict  
564 MPR for media with  $H=0.1$  and  $H=0.5$ , respectively. Grey dashed lines are plotted to facilitate the MPR  
565 comparison in two nearby panels. Wavefield scattering is proportional to the standard deviation of  
566 medium heterogeneities, and inversely proportional to correlation length for large Hurst exponent ( $H=$   
567  $0.5$ ), but remains nearly unaffected by variations in correlation length for small Hurst exponent ( $H= 0.1$ ).  
568 The  $k_w a$  maxima for correlation lengths of 1, 5 and 10 km are 9.07, 45.36 and 90.72, respectively.

569

570 **Figure 4:** Mean PGA ratios (MPR) for eight numerical simulations as a function of distance, depicting the  
571 effects of wavefield scattering on ground-motions in the regime  $k_w a \approx 1$ . Panels (a) and (b) depict MPR  
572 for media with  $H=0.1$  and  $H=0.5$ , respectively. Grey dashed lines are plotted to facilitate the MPR  
573 comparison in two nearby panels. Wavefield scattering is proportional to correlation length, Hurst  
574 exponent, and standard deviation of medium heterogeneities. The highest values of  $k_w a$  for correlation  
575 lengths of 1 and 5 km are 0.90 and 4.53, respectively.

576

577 **Figure 5:** Mean PGA ratios (MPR) for all eight numerical simulations as a function of distance, depicting  
578 the effects of wavefield scattering on ground-motions in the regime  $k_w a \ll 1$ . Panels (a) and (b) depict  
579 MPR for media with  $H=0.1$  and  $H=0.5$ , respectively. Grey dashed lines are plotted to facilitate the MPR  
580 comparison in two nearby panels. Wavefield scattering is proportional to correlation length, Hurst

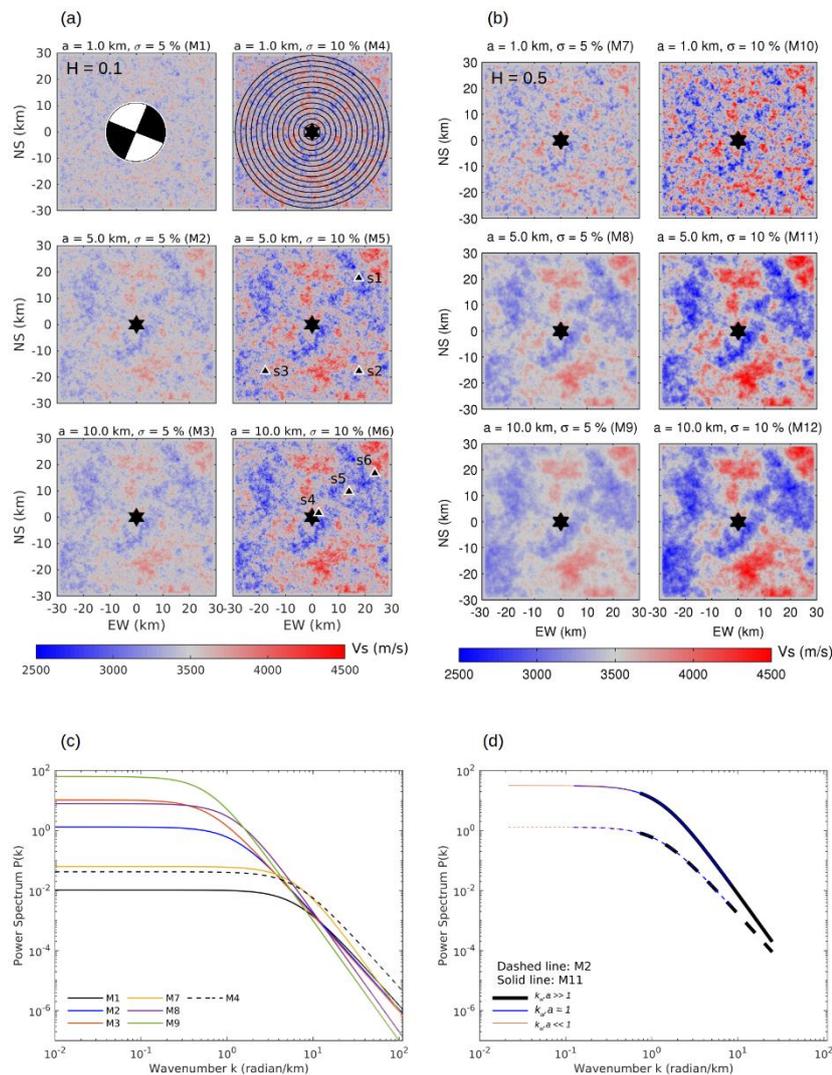
581 exponent, and the standard deviation of medium heterogeneities. The highest values of  $k_w a$  for  
582 correlation lengths of 5 and 10 km are 0.27 and 0.54, respectively.

## List of Tables

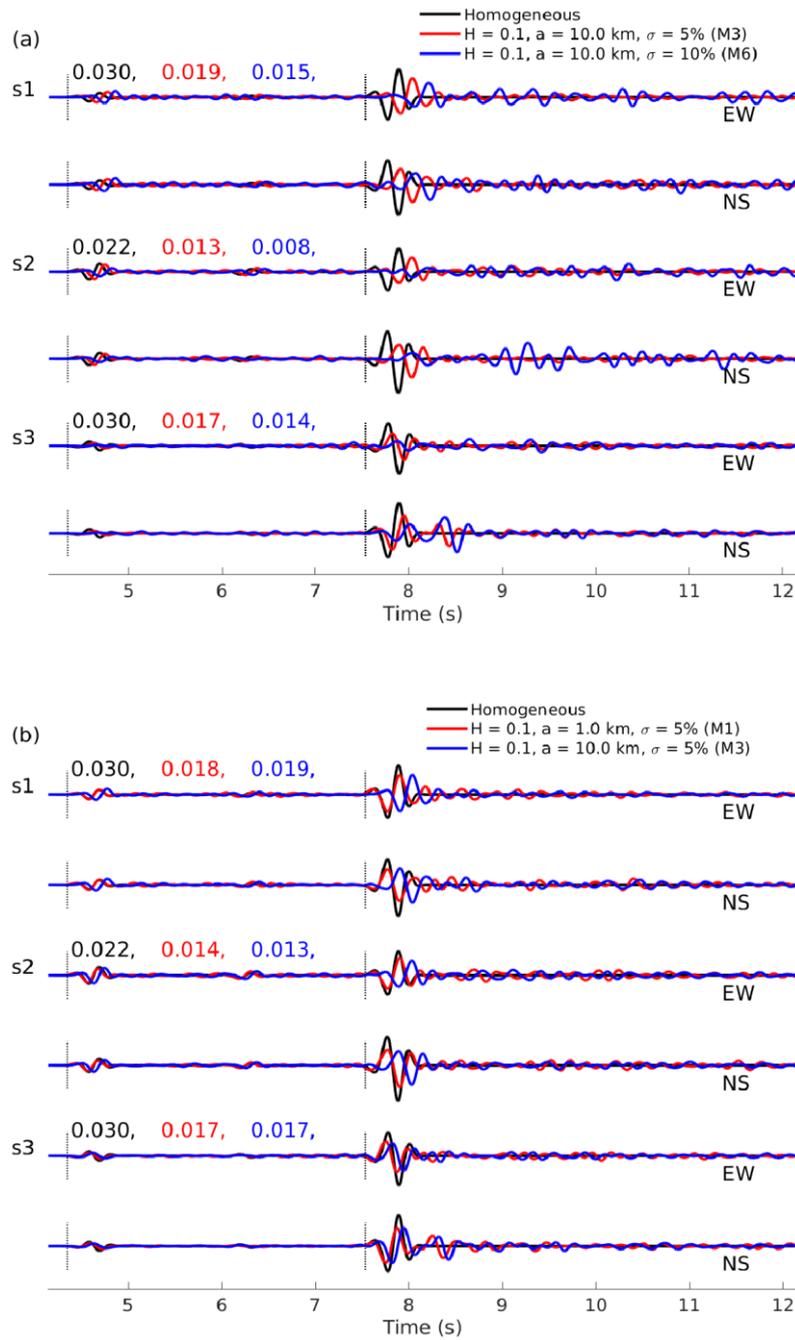
<b>Table 1:</b> Parameters for the 28 computational 3D Earth models generated for this study.			
Model Reference	Correlation length $a$ (km)	Standard deviation $\sigma$ (%)	Hurst exponent $H$
M1, M1-L	1.0	5	0.1
M2, M2-L, M2-EL	5.0	5	0.1
M3, M3-EL	10.0	5	0.1
M4, M4-L	1.0	10	0.1
M5, M5-L, M5-EL	5.0	10	0.1
M6, M6-EL	10.0	10	0.1
M7, M7-L	1.0	5	0.5
M8, M8-L, M8-EL	5.0	5	0.5
M9, M9-EL	10.0	5	0.5
M10, M10-L	1.0	10	0.5
M11, M11-L, M11-EL	5.0	10	0.5
M12, M12-EL	10.0	10	0.5

Parameters of 28 computational 3D models generated using random fields characterized by von Karman autocorrelation functions (parametrized by correlation length, standard deviation and Hurst exponent). The suffixes “-L” and “-EL” indicate large and extra-large models, respectively.

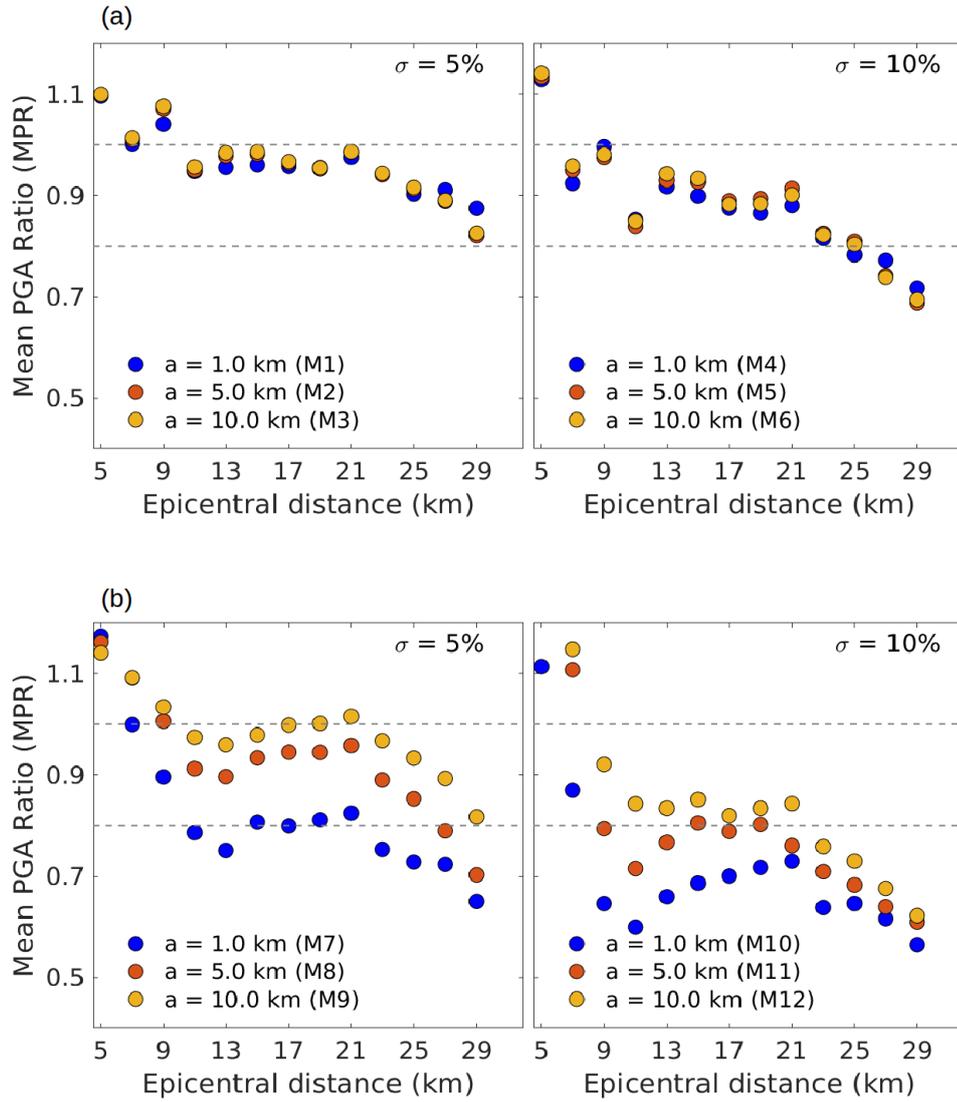
## List of Figures



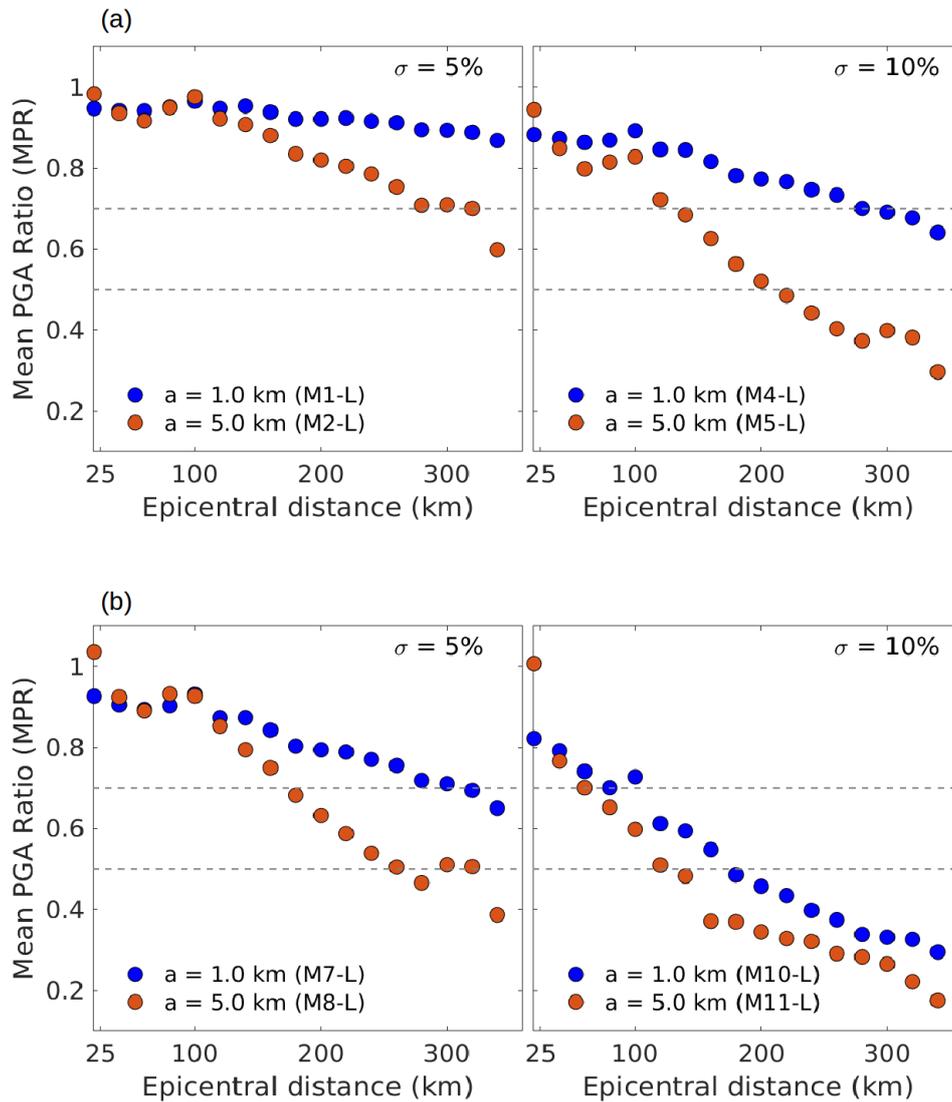
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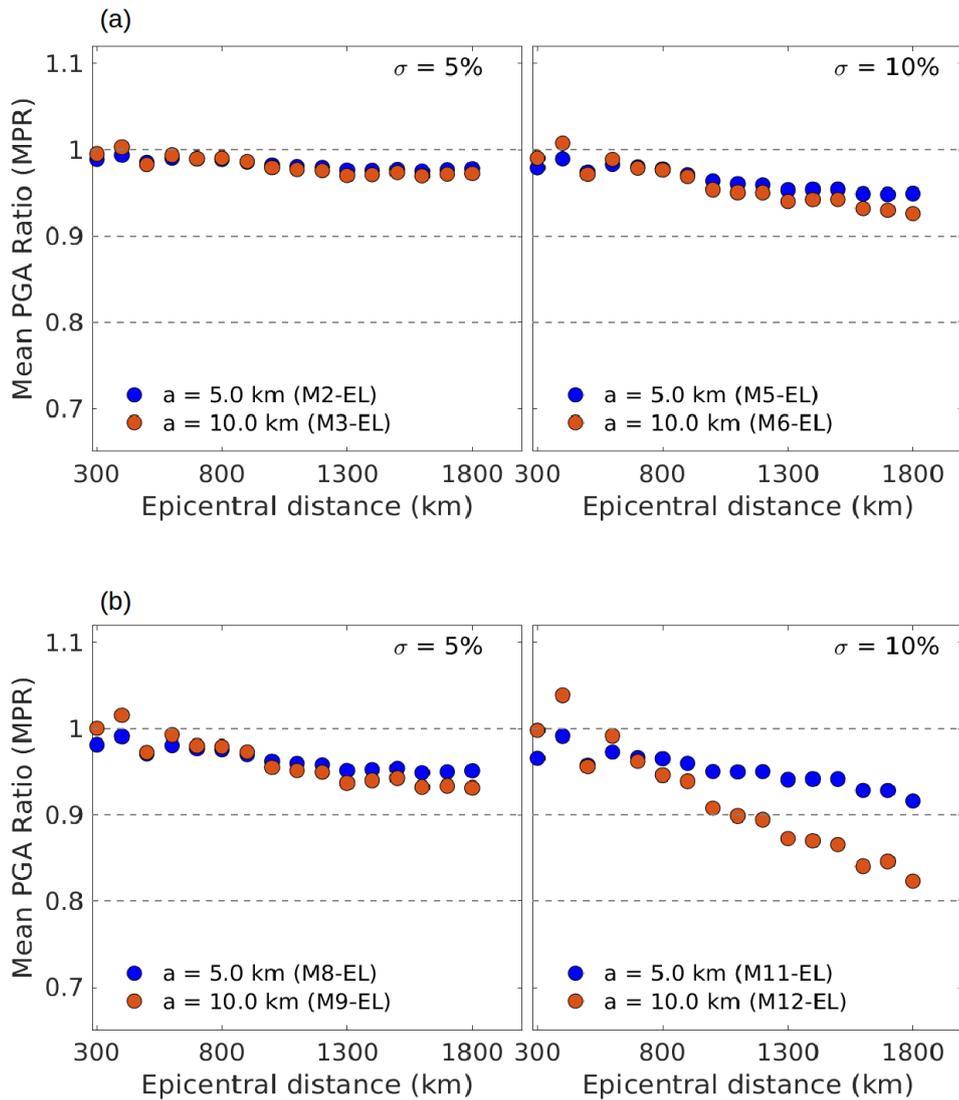
**Figure 2:** Horizontal components (East-West, EW, and North-South, NS) of ground acceleration ( $\text{m/s}^2$ ) at sites s1, s2, s3 (Fig 1a). Black dotted lines indicate theoretical P- and S-wave arrival times in the considered homogeneous medium. Color-coded numbers indicate PGA values at individual sites. Waveforms are normalized by their PGA-value in the homogeneous-medium simulations for a given site. (a) Illustration of scattering controlled by  $\sigma$  for  $k_w a \gg 1$  and small  $H$ ; (b) Illustration of negligible effects of correlation length on scattering for  $k_w a \gg 1$  and small  $H$ .



**Figure 3:** Mean PGA ratios (MPR) for all twelve numerical simulations as a function of distance, depicting the effects of wavefield scattering on ground-motions in the regime  $k_w a \gg 1$ . Panels (a) and (b) depict MPR for media with  $H=0.1$  and  $H=0.5$ , respectively. Grey dashed lines are plotted to facilitate the MPR comparison in two nearby panels. Wavefield scattering is proportional to the standard deviation of medium heterogeneities, and inversely proportional to correlation length for large Hurst exponent ( $H=0.5$ ), but remains nearly unaffected by variations in correlation length for small Hurst exponent ( $H=0.1$ ). The  $k_w a$  maxima for correlation lengths of 1, 5 and 10 km are 9.07, 45.36 and 90.72, respectively.



**Figure 4:** Mean PGA ratios (MPR) for eight numerical simulations as a function of distance, depicting the effects of wavefield scattering on ground-motions in the regime  $k_w a \approx 1$ . Panels (a) and (b) depict MPR for media with  $H=0.1$  and  $H=0.5$ , respectively. Grey dashed lines are plotted to facilitate the MPR comparison in two nearby panels. Wavefield scattering is proportional to correlation length, Hurst exponent, and standard deviation of medium heterogeneities. The highest values of  $k_w a$  for correlation lengths of 1 and 5 km are 0.90 and 4.53, respectively.



**Figure 5:** Mean PGA ratios (MPR) for all eight numerical simulations as a function of distance, depicting the effects of wavefield scattering on ground-motions in the regime  $k_w a \ll 1$ . Panels (a) and (b) depict MPR for media with  $H=0.1$  and  $H=0.5$ , respectively. Grey dashed lines are plotted to facilitate the MPR comparison in two nearby panels. Wavefield scattering is proportional to correlation length, Hurst exponent, and the standard deviation of medium heterogeneities. The highest values of  $k_w a$  for correlation lengths of 5 and 10 km are 0.27 and 0.54, respectively.