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De la propagation à la diffusion des ondes dans les solides : apports et limites de la simulation numérique.

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Résumé — La propagation d'ondes dans des solides hétérogènes propose des défis redoutables à la modélisation numérique. Citons par exemple les phénomènes de guidage, de diffraction simple ou multiple, de diffusion ou de localisation ; les radiations à l'infini, la prise en compte de l'aléa du milieu, la disparité des échelles ou l'effet de la dimension spatiale dans la sélection des régimes de propagation. Aux limites liées à la taille des modèles numériques s'ajoute la difficulté de la validation, cette dernière ne pouvant souvent s'envisager qu'en comparaison à des modèles limites théoriques : transfert radiatif, diffusion, champ moyen ou des propriétés remarquables telles que l'égalité de Ward ou le renversement temporel.

Nous évoquons dans cet article les apports et limites de différentes techniques numériques : éléments spectraux, éléments de frontière, différences finies, frontières absorbantes et ouvrons des perspectives sur les couplages entre modèles de propagation en milieu aléatoire et modèles de transfert radiatif.

Mots clés — Ondes élastiques, diffraction, milieux aléatoires, éléments finis, transfert radiatif.

1 Introduction

Numerical modelling of wave propagation has been a challenging issue for decades. Indeed several scales have to be dealt with continuously increasing the computational demand. When piecewise homogeneous media are at stake the ratio between the propagation distance L and the wavelength λ is the main parameter governing the propagation regime from low to high frequencies. The main difficulties are (i) the account of the boundary conditions, (ii) the restriction to a finite size computational domain, (iii) the dispersion of the numerical scheme both in time and space. Hopefully, many analytical solutions are available to assess the quality of any numerical scheme in all these regimes.

From the numerical point of view, several methods have been competing up to now to overcome these difficulties and reach both quality and computational efficiency. The Finite Difference Method was the first to achieve significant results in the high frequency range mainly with the introduction of a staggered grids [21] to prevent the dispersion of the wavefield. However complex boundary conditions are still difficult to account for in this method, together with a strong heterogeneity of the medium. The Finite Element Method had often been considered less efficient than the FD one and had been reported to yield strong wave dispersion at high frequencies [3] especially for low order elements. These two drawbacks have been overcome taking higher order elements with lumped mass matrices as done in Spectral Finite Elements [13, 9]. The remaining difficulty of domain truncation both shared by the FD and FE methods has been dealt with by means of absorbing boundary conditions or more efficiently by Perfectly Matched Layers [5]. Before these recent developments, Boundary Element Methods had often provided the most accurate solutions together with a good efficiency for low to medium frequency problems. Multipole methods [7] have tremendously increased their efficiency allowing to deal with analyses involving several tenth of wavelengths. However these methods are basically restricted to locally homogeneous isotropic domains even though special developments have been done to account for layered media [8].

Yet, despite these significant developments, the ability of these methods to model accurately the propagation of waves over a large number of wavelengths throughout a strongly heterogeneous medium is still an open question. From the practical point of view, numerical solutions computed on large scale models with piecewise homogeneous material are known to significantly overestimate the dynamic response. The discrepancy can be minimized adding some material damping in the model but it is known for long [1] that this equivalent damping is actually due to multiple scattering. The energy lost in the

early arrivals is transferred to the later ones. Moreover the decay of the energy of these late arrivals in the signal is known to be related to the statistical properties of the heterogeneous propagation medium. Hence two additional characteristic distances enter the picture : ℓ_c the correlation length on the physical properties and the mean free path ℓ_t -the mean distance over which a wave is scattered once.

The question we address here is to know whether the above mentioned numerical methods are able to accurately model these phenomena without adding uncontrolled numerical dispersion. It is an involving question since, except for some periodic cases which are only relevant in very specific cases, no analytical solutions are available to assess this efficiency. Moreover, *prior* error estimates, although quite valuable to build numerical models, are often too coarse to assert their accuracy. Yet both theoretical and experimental research works in the field of wave in random media have produced many interesting results to this aim. It is believed that the ability of numerical models to simulate peculiar properties such time reversal refocusing and asymptotic behaviours such as diffusion regimes could be good indicators on their accuracy. In addition it would also be a way to identify the range of validity of these asymptotic solutions. Finally it would provide valuable insights into the required amount of information needed to describe the heterogeneous media. Methods to invert these properties from experimental data could also benefit from these results.

In order to achieve this goal, a model for a random anisotropic elastic medium controlled by a reduced number of parameters is need. This model is derived from a maximum entropy principle with given mean properties, fluctuation level and correlation length. Since the Soize's model of non-gaussian positive-definite matrix-valued random field of minimal parameterization [18] shows a linear increase of the fluctuation level with the mean anisotropy index [6, 19] independent controls on these two parameters have been proposed in [19] and are briefly described in section 2. Another control on the anisotropy level based on the mean distances of the elastic tensor eigenvalues have been proposed in [12].

The second ingredient is an efficient and accurate elastodynamic numerical solver for strongly heterogeneous and anisotropic unbounded media. The Spectral Element Method [13] coupled with Domain Decomposition techniques and Perfectly Matched Layers [5] have been chosen to this aim. More specifically we used the SPEC3D software developed at IGP for applications in geophysics [9]. A generator of random elastodynamic fields based on the spectral representation theorem had been implemented together with modified PML [19] in order to eliminate the instability of standard PMLs for anisotropic elastic properties [4].

Section 4 gives some preliminary validation results of two types. Time-reversal properties of the numerical scheme are first analysed showing the accuracy of the model. Then the model ability to reach the diffusion regime at large time is investigated in terms of energy equipartition. These results show that this regime is actually reached for strongly fluctuating anisotropic media. A scaling law between the mean transport time - the time after which diffusion is reached- and the correlation length of the medium is identified. On the contrary, it is shown that for strongly fluctuating isotropic properties such a diffusion regime does not show up in the numerical simulations suggesting that another phenomenon can be at stake.

2 Probabilistic model of elastic property fields

In the section we first concentrate on the probabilistic modeling of an elastic tensor. The aim is to write this tensor as a known non-linear transform of a set of Gaussian random variables. Equipped with this transform a random field of elastic tensor can easily be defined in a second step as a non linear transform of a Gaussian random fields.

2.1 Random elastic tensor

The linear elastic behavior of a material is characterized by the elasticity tensor \mathbf{C} , linking the stress tensor $\boldsymbol{\sigma}$ and the strain tensor $\boldsymbol{\epsilon}$. The Voigt's notation is used to replace this 4-rank tensor by a 2-rank symmetric positive-definite matrix with 21 independent coefficients for general anisotropic materials. When the material shows local symmetries the number of independent coefficients decreases and reduces to 2 independent coefficients in the isotropic case. Among other choices of that pair of coefficients, the

tensor \mathbf{C}^{iso} of an isotropic material can be written using the bulk modulus κ and shear modulus μ :

$$\mathbf{C}^{iso} = 3\kappa\mathbf{S} + 2\mu\mathbf{D} \quad (1)$$

where \mathbf{S} and \mathbf{D} are respectively the so-called *spherical* tensor and *deviatoric* tensor defined as : $\mathbf{S} = \frac{1}{3}(\mathbf{I}_2 \otimes \mathbf{I}_2)$ and $\mathbf{D} = \mathbf{Id}_6 - \mathbf{S}$ with $\mathbf{I}_2 = [1 \ 1 \ 1 \ 0 \ 0 \ 0]^T$ and \mathbf{Id}_6 the identity matrix of $\mathbb{M}_6(\mathbb{R})$. Since $\{\mathbf{S}, \mathbf{D}\}$ are orthogonal projectors in the space of real symmetric matrices $\mathbb{M}_6^s(\mathbb{R})$ ($\mathbf{S}^2 = \mathbf{S}$, $\mathbf{D}^2 = \mathbf{D}$ and $\mathbf{SD} = 0$) and an orthogonal pair for the scalar product associated to the Frobenius norm ($\|\mathbf{S}\|_F = 1$; $\|\mathbf{D}\|_F = \sqrt{5}$), equation [1] also reads :

$$\mathbf{C}^{iso} = \left(\sqrt{3\kappa}\mathbf{S} + \sqrt{2\mu}\mathbf{D} \right)^2 \quad (2)$$

Based on equation [2], we propose to write a random anisotropic elasticity tensor as :

$$\mathbf{C}(\delta, \delta_g) = \left(\sqrt{3\kappa(\delta)}\mathbf{S} + \sqrt{2\mu(\delta)}\mathbf{D} \right) \mathbf{G}(\delta_g) \left(\sqrt{3\kappa(\delta)}\mathbf{S} + \sqrt{2\mu(\delta)}\mathbf{D} \right) \quad (3)$$

in which $\mathbf{G}(\delta_g)$, $\kappa(\delta)$ and $\mu(\delta)$ are random variables and (δ, δ_g) a pair of dispersion parameters.

Following [18], the so-called anisotropy kernel \mathbf{G} belongs to the set SG^+ of all normalized, symmetric, positive-definite real random matrices. This random variable is defined on the probability measure space $(\mathcal{A}, \mathcal{F}, P)$, with values in $\mathbb{M}_6^+(\mathbb{R})$, parameterized by a unique real positive dispersion parameter δ_g . According to [17], the construction by maximizing the entropy leads to the following form of the kernel :

$$\mathbf{G}(\delta_g) = \mathbf{L}^T(\delta_g)\mathbf{L}(\delta_g) \quad (4)$$

where \mathbf{L} is an upper triangular matrix whose diagonal coefficients are gamma distributed and extra-diagonal coefficients are Gaussian. As far as random isotropic elasticity moduli are concerned, the bulk and shear moduli are modeled as independent strictly positive real random variables. Applying the maximum entropy principle with given mean values $(\underline{\kappa}, \underline{\mu})$ and mean logarithm, leads to two *Gamma* distributed random variables which can be easily mapped to two independent copies of the Gaussian scalar variable using the iso-probability transformation. It is worth noticing that other probability laws such as lognormal could have been chosen, together with correlations between these two gaussian germs.

Properties of matrix-valued random variable \mathbf{C}

Thanks to the knowledge of $\kappa(\delta)$, $\mu(\delta)$ and $\mathbf{G}(\delta_g)$, the random elastic tensor $\mathbf{C}(\delta; \delta_g)$ defined in equation [3] has the following properties as shown in [20] :

- (i) $\mathbf{C}(\delta; \delta_g)$ has an isotropic mean given by : $\underline{\mathbf{C}} = 3\underline{\kappa}\mathbf{S} + 2\underline{\mu}\mathbf{D}$
- (ii) $\mathbf{C}(\delta, \delta_g)$ is a second order random variable : $E \{ \|\mathbf{C}(\delta, \delta_g)\|_F^2 \} < +\infty$
- (iii) $\mathbf{C}^{-1}(\delta, \delta_g)$ is a second order random variable when : $\delta^2 < \frac{1}{2}$ and $\delta_g^2 < \frac{7}{11}$
- (iv) The anisotropy level is linearly controlled by δ_g .
- (v) The global fluctuation of the norm of $\mathbf{C}(\delta, \delta_g)$ depends explicitly on δ_g and δ as :

$$\delta_{|C|}^2 = \frac{E \{ \|\mathbf{C} - \underline{\mathbf{C}}\|_F^2 \}}{\|\underline{\mathbf{C}}\|_F^2} = \delta^2 + \frac{\delta_g^2}{7} \left(1 + \frac{\text{tr}^2(\underline{\mathbf{C}})}{\|\underline{\mathbf{C}}\|_F^2} \right) \quad (5)$$

As far as the anisotropy level is concerned, several measures can be defined [6]. It is shown in [19] that the mean anisotropy index I_a defined as the mean square distance between $\mathbf{G}(\delta_g)$ and its projection on the isotropic subspace of $\mathbb{M}_6^+(\mathbb{R})$ and normalized by the square of the norm of the mean value of \mathbf{G} :

$$I_a = \sqrt{\frac{E \{ \|\mathbf{G} - \bar{\mathbf{C}}\|_F^2 \}}{6}} \quad (6)$$

is explicitly controlled by the parameter δ_g as :

$$0 \leq I_a = \sqrt{\frac{19}{21}}\delta_g \leq \sqrt{\frac{19}{33}} < 0.76 \quad (7)$$

Based in numerical simulations, it is shown [19] to be equivalent to the standard mean index.

2.2 Stochastic field of elasticity tensor

Up to now, only the variability of the elasticity tensor at a given point has been accounted for. In order to introduce the spatial variability of this mechanical property, the present section discusses the construction of a model of the stochastic field of elasticity tensor based on the probabilistic model developed in the previous section. Let $\Omega = \{\mathbf{x} | \mathbf{x} \in \mathbb{R}^3\}$ be the physical domain, equipped with a Cartesian reference frame $\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$, and occupied by an inhomogeneous elastic material. The associated stochastic field model of elasticity tensor $\{\mathbb{C}(\boldsymbol{\delta}; \boldsymbol{\delta}_g; \boldsymbol{\ell}) | \mathbf{x} \in \Omega\}$, defined on the probability measure space $(\mathcal{A}, \mathcal{F}, P)$, indexed on Ω , with values in $\mathbb{M}_6^+(\mathbb{R})$, can then be formulated as follows :

$$\left\{ \mathbb{C}(\mathbf{x}; \boldsymbol{\delta}, \boldsymbol{\delta}_g; \boldsymbol{\ell}) = \left(\sqrt{3\kappa(\mathbf{x}; \boldsymbol{\delta}; \boldsymbol{\ell})} \mathbf{S} + \sqrt{2\mu(\mathbf{x}; \boldsymbol{\delta}; \boldsymbol{\ell})} \mathbf{D} \right) \mathbf{G}(\mathbf{x}; \boldsymbol{\delta}_g; \boldsymbol{\ell}) \right. \\ \left. \left(\sqrt{3\kappa(\mathbf{x}; \boldsymbol{\delta}; \boldsymbol{\ell})} \mathbf{S} + \sqrt{2\mu(\mathbf{x}; \boldsymbol{\delta}; \boldsymbol{\ell})} \mathbf{D} \right) \right\} \text{ a.s.} \quad (8)$$

where $\boldsymbol{\ell} = (\ell_1, \ell_2, \ell_3)$ is a vector of correlation lengths in the three spatial directions. The evolution from equation [3] to equation [8] is done by replacing, in the formulation of the kernel \mathbf{G} and of the isotropic elastic modulus κ, μ , the 23 independent copies $\{\mathcal{G}_k | k \in \{1, 2, \dots, 23\}\}$ of a Gaussian normalized random variable by 23 independent copies $\{\mathcal{G}_k(\mathbf{x}; \boldsymbol{\ell}) | \mathbf{x} \in \Omega; k \in \{1, 2, \dots, 23\}\}$ of a stochastic Gaussian field $\{\mathcal{G}(\mathbf{x}; \boldsymbol{\ell}) | \mathbf{x} \in \Omega\}$ indexed on Ω with values in \mathbb{R} . This germ Gaussian field is of second-order, homogeneous with a correlation defined by a spectral density with bounded support (see, [18, 2], for more details). This stochastic field $\{\mathbb{C}(\mathbf{x}; \boldsymbol{\delta}, \boldsymbol{\delta}_g; \boldsymbol{\ell})\}$ is mean-square continuous with almost surely continuous samples. Following [18], it can be shown that taking the restriction of this field on a bounded domain leads to a second order solution of the related stochastic boundary value problem. Finally it can be sample using standard spectral simulation [16].

3 Numerical model

Since the goal is to characterize the wave propagation pattern in a random media beyond the *mean free path*, it requires a numerical method able to account for several wavelengths and correlation lengths in all spatial directions. Moreover, since the multiple scattering pattern drastically changes between two and three dimensional cases, 3D simulations are targeted. In order to meet both a high efficiency and a controlled numerical error, the Spectral Finite Element Method has been chosen. In particular, the SPEC software developed by the Seismology Group of *Institut de Physique du Globe de Paris* [9] has been modified in order to account for anisotropic heterogeneous fields of elastic tensors. It is worth noticing that in this paper only samples of random medium will be considered and no real statistical analyses will be performed. However, since the elastic waves are traveling through a statistically homogeneous random medium, the wave pattern obtained after several wavelengths and correlation lengths is expected to show common statistical properties almost independent of the sample.

The strong formulation of the elastic wave propagation in an anisotropic media Ω consists in solving for \mathbf{u} the Navier equation $\forall t \in [0; T]$:

$$\text{Div}(\mathbf{C}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{u}(\mathbf{x}; t))) + \mathbf{f}(\mathbf{x}, t) = \rho_v \frac{\partial^2}{\partial t^2} \mathbf{u}(\mathbf{x}; t) \quad (9)$$

together with proper boundary and initial conditions. \mathbf{C} is a sample of the random field of anisotropic elastic tensor and ρ_v is the bulk density. As far as the Spectral Finite Element Method is concerned, the related weak formulation is considered $\forall t \in [0; T]$ and $\forall \mathbf{w} \in V(\Omega)$:

$$\int_{\Omega}^* \left(\rho_v \frac{\partial^2 \mathbf{u}}{\partial t^2}(t) \cdot \mathbf{w} + \mathbf{C}^*(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{u}(t)) : \boldsymbol{\varepsilon}(\mathbf{w}) - \mathbf{f}(\mathbf{x}, t) \cdot \mathbf{w} \right) d\Omega = 0 \quad (10)$$

where $\mathbf{C}^* = \mathbf{C}$ in the domain of interest Ω and where \mathbf{C}^* corresponds to a modified integro-differential operator with respect to time inside the PML $\Omega^* \setminus \Omega$. Indeed, the PML can be viewed as an anisotropic dispersive material. In addition, it is worth noticing that such PML are applicable to inhomogeneous media but can become instable for anisotropic materials [4]. As a consequence, they have to be modified using either a projection of the anisotropic tensor in the PML on the isotropic subspace or a multiaxial

damping [11] leading to stable but not perfectly matched layers. This is a significant drawback when homogeneous material are sought for. It is less important for strongly inhomogeneous media since perfectly or non perfectly matched layers are both unsuited in this case. The development of equivalent boundary conditions in such media is still a pending question.

4 Validation and preliminary results

The aim of this section is to give elements to the validation of the numerical model for wave propagation in strongly fluctuating media with correlation lengths of the order of the wavelength. It is first done in terms of time reversal properties of the numerical scheme and then in terms of capability of reaching asymptotic diffusion regimes at large time. Besides, the proposed results will allow to related properties of the wave field, namely the so-called *transport mean free time* after which the diffusion regime is reached and the parameters of the elastic property random field.

4.1 Validation of time reversal properties of the numerical scheme

Time reversal is an obvious property of any linear wave equation. When applied to random media, it leads to a rather counterintuitive result : a complex scattered field spreading on a very large domain can be refocused on the source. From the experimental point of view, it has been shown that this feature can be reproduced accurately and that the quality of refocussing is even better when the propagation medium shows strong fluctuations [10]. From the numerical point of view, time reversal simply consists in changing the sign of the velocity field at all points and at a given time step and let the time marching scheme proceed. It is believed that this procedure and the quality of the refocussing achieved is a good indicator on the time and space dispersion of the numerical scheme.

From the theoretical point of view the refocussing should be perfect when Neumann boundary conditions are applied on the boundary of the computational domain as actually observed in figure 1. When PMLs are used, errors are expected since time reversal does not apply inside the PML. However the refocussing properties are preserved as shown in figure 1.

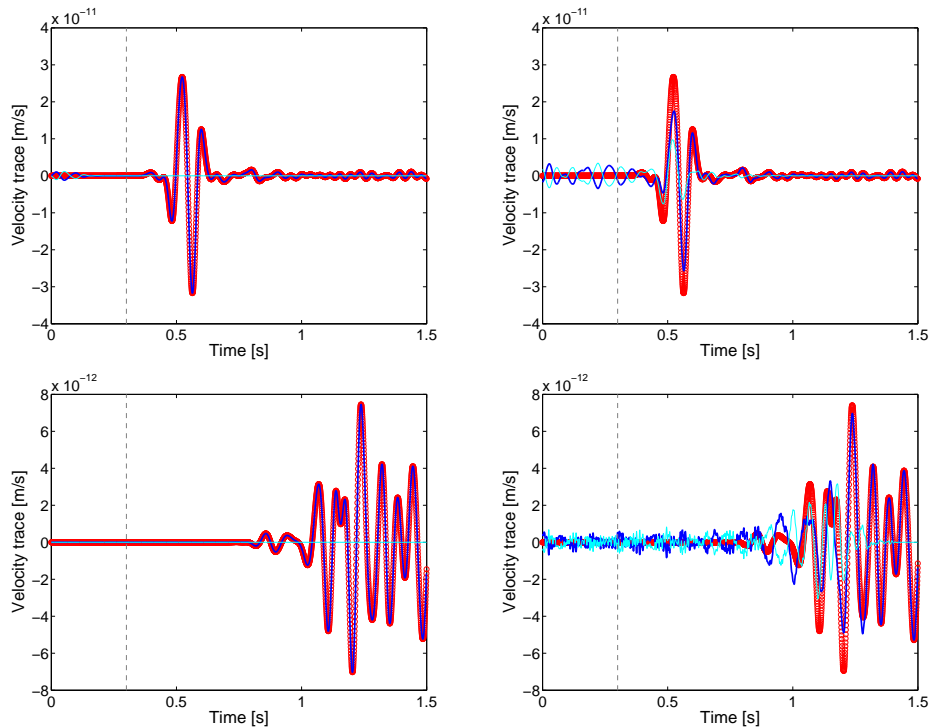


FIGURE 1 – Direct (red), reversal (dark blue) and error (light blue) time histories of the velocity field on the free surface of a random elastic medium for Neumann boundary condition (left) and PMLs (right), at 200m (top) and 800m (bottom) from the source.

4.2 Diffusion regime

From both theoretical and experimental results [15, 14], it is known that a wave field in a weakly fluctuating medium reaches a diffusion regime. This regime is characterized by an equipartition of the energy between all propagation modes : i.e. in terms of wave polarization and propagation direction. Given a localized source, the time needed to reach this regime is denoted by τ_t and is proportional to the *transport mean free path* ℓ_t . This *transport mean free time* τ_t is expected to decrease with the fluctuation level and to increase with the correlation length ℓ_c . However closed-form solutions of these relationships are only available for small fluctuation and isotropic media.

Diffusion regime for isotropic and anisotropic random media

The assumption that a diffusion regime is always reached and that, given a correlation model for the medium, the *transport mean free time* is governed by the fluctuation level $\delta_{|C|}$ seems questionable. Indeed figure 2 shows the comparison between the wavefield obtained inside two random media having the same correlation model and the same fluctuation level $\delta_{|C|}$, one being isotropic and the other anisotropic. It is quite obvious that when in the anisotropic case the diffusion regime is reached. It is not true in the isotropic case where the wavefield is localized on some weak zones of the medium.

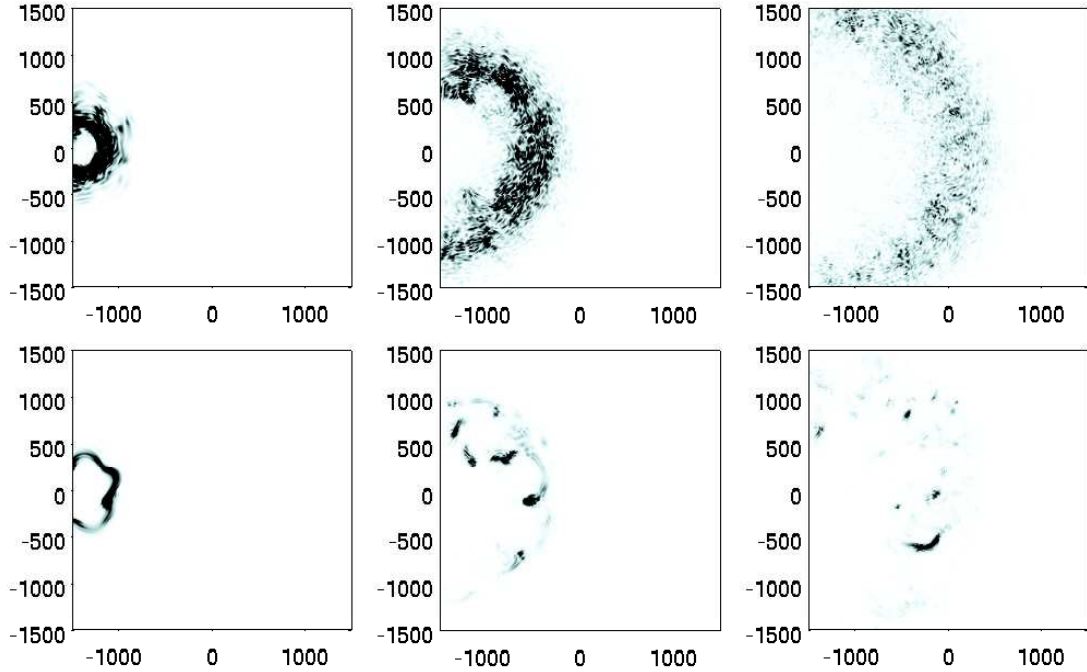


FIGURE 2 – Time evolution of wavefronts on the free surface for $\delta_{|C|} = 0.49$: (top) $\delta = 0; \delta_g = 0.6$, (bottom) $\delta = 0.47; \delta_g = 0.17$ (A full description of the model can be found in [19]).

Estimates of the transport mean free time

A quantitative evaluation of the *transport mean free time* can be obtained observing the equipartition property. In the case of an isotropic medium it is characterized by a constant ratio between the P-wave and S-wave energies with respect to time. For weak fluctuations this ratio tends to an explicit limit [15] depending on the P and S wave velocities c_P and c_S :

$$\lim_{t \gg \tau_t} \frac{\mathcal{E}_P}{\mathcal{E}_S} = \frac{1}{2} \left(\frac{c_S}{c_P} \right)^3, \quad \mathcal{E}_P = \left(\frac{\lambda}{2} + \mu \right) (\text{Div} \mathbf{u})^2, \quad \mathcal{E}_S = \mu \|\text{rot} \mathbf{u}\|^2 \quad (11)$$

with λ and μ the two lamé coefficients. The value of this limit is not known for an anisotropic case where even the definition of P-wave and S-wave energy is questionable. However, since the random media of concern have an isotropic mean elastic tensor, it is believed that this property holds in the mean sense. Hence we have proposed in [19] to compute the average of this ratio on the entire computational domain

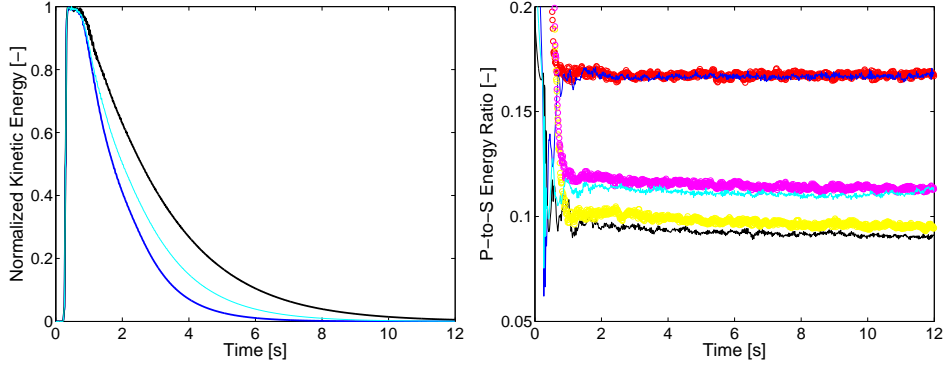


FIGURE 3 – Comparison between three random media having the same correlation length and fluctuation level $\delta_C = 0.6$: $\delta = 0.6$ (black and yellow); $\delta_G = 0$, $\delta = 0$ (dark blue and red); $\delta_G = 0.6476$ and $\delta = 0.5$ (light blue and purple); $\delta_G = 0.3327$. (left) The total energy as a function of time for a shear source (right) The energy ratio for shear (continuous lines) and explosive sources (circles).

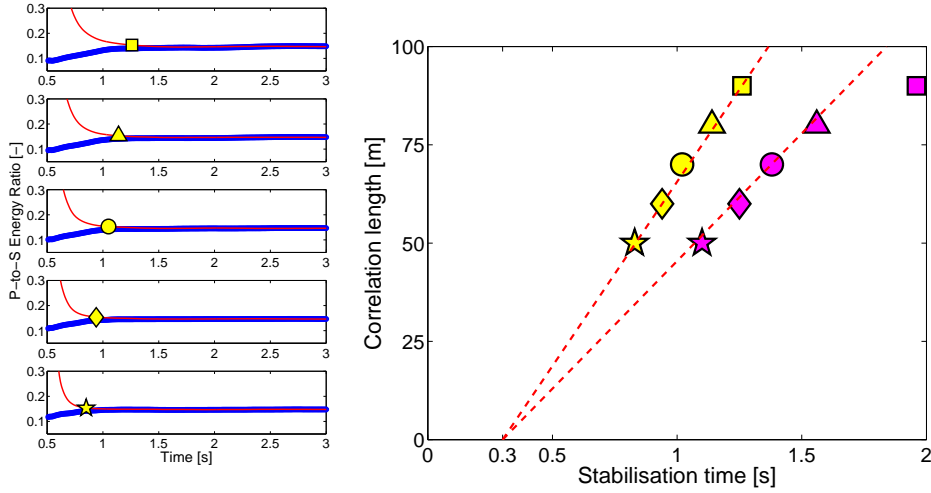


FIGURE 4 – Stabilisation of the energy ratio for $\delta = 0$, $\delta_G = 0.5387$ (left) and from top to bottom $l_c = 90\text{m}$, $l_c = 80\text{m}$, $l_c = 70\text{m}$, $l_c = 60\text{m}$ and $l_c = 50\text{m}$; (right) stabilisation time as a function of the correlation length for $(\delta = 0; \delta_G = 0.5387)$ and $(\delta = 0; \delta_G = 0.4317)$.

using at each point the Lamé coefficients λ^{eqv} and μ^{eqv} of the closest isotropic elastic material to the local anisotropic one. This energy ratio is plotted in figure 3 for isotropic and anisotropic random media having the same fluctuation level and correlation length together with the decay of the total energy with respect to time. It can easily be noticed that when the energy ratio reaches rapidly a constant value in the strongly anisotropic case, it does not converge at large time for the isotropic and weakly anisotropic cases. The slower decay of the energy in these latter cases indicates that the energy tends to remain trapped in the medium. Hence the diffusion limit for large fluctuation levels is only reached in the strongly anisotropic case. In this case a *transport mean free time* can easily be identified. It is the time at which the convergence is reached. This *transport mean free time* can be identify for several correlation lengths and several fluctuation levels as shown in figure 4. It is observed that this *transport mean free time* is proportional to the correlation length and increase when the fluctuation level increases as expected.

5 Conclusions

Several tools to validate numerical simulations of elastic wave propagation in random anisotropic media have been proposed including time reversal simulation and the identification of a *transport mean free time* after which diffusion regimes are observed. These techniques have been shown to be quite effective for high fluctuation level and strong anisotropy. In particular the *transport mean free time* has been shown to be proportional to the wavelength and a decreasing function of the fluctuation level. It has

also been observed that such a diffusion regime has not been reached for large fluctuation of an isotropic medium due the localization of waves. Hence additional and more expensive computations have to be performed for smaller fluctuation levels to retrieve classical asymptotic results.

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