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Energy based a posteriori analysis for finite element modeling of elastic wave propagation in heterogeneous media

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Abstract — This work deals with a posteriori quality control for FE modeling of high frequency wave propagation in heterogeneous media. Special attention should be paid here in the definition of numerical models to ensure accuracy of solutions and optimality of computation costs. Herein, we propose to qualify the numerical waves in terms of energy densities governed by radiative transfer equations, obtained by a multi-scale asymptotic analysis and Wigner transforms. Radiative transfer residuals of FE wave solutions are used to build a posteriori error analysis.
Keywords — a posteriori quality control, Wigner transform, energy quantity, radiative transfer equation.

1 Introduction

In heterogeneous or random media, strong interactions between waves and such media generate complex phenomena. After a large number of scattering, the wave fields become stochastic and wave field cannot be represented by any coherent plane wave. An mean quadratic quantity such as energy density is more meaningful for a posteriori analysis. So the Wigner transform in the phase space is introduced and it resolves the wave energy locally over all possible directions. It allows to derive a radiative transfer equation which describes the transport and scattering of wave energy in heterogeneous media. The key idea of our approach is instead of solving directly this radiative transfer equation, the Wigner transform of the finite element solutions of the elastic wave equation is calculated and analyzed by considering the residuals with respect to the radiative transfer equation.

In this paper, we will firstly introduce the elastic wave equation and the definition of Wigner transform and its non negative weak limit; then we derive the radiative transfer equation in different cases; the residual errors are developed in one dimensional case and its numerical applications in 1D homogeneous and heterogeneous are given in the end.

2 Elastic wave propagation in a high-frequency setting

In this section we will introduce the HF wave propagation for the derivation of the radiative transfer equation. The main notations and definitions are also presented here.

2.1 Elastic wave equation

We consider HF wave propagation in random media in weak coupling regime, which means that the wavelength λ is small compared to the propagation distance L and the correlation length of the weak random inhomogeneities l is of the same order as the wavelength λ. The displacement field is denoted by $\mathbf{u}_\varepsilon(t,\mathbf{x})$ and its second order Cauchy stress tensor is denoted by $\sigma_\varepsilon(t,\mathbf{x})$. The subscript ε is defined as a new spatial(temporal) scale: $\varepsilon \sim \frac{\lambda}{L}$, and we introduce two spatiotemporal scales: slow one $(t,\mathbf{x})$ and fast one $(t/\varepsilon, \mathbf{x}/\varepsilon)$.

We consider here a two order wave equation in an open domain Ω as follows:

$$\rho(\mathbf{x})\partial_t^2\mathbf{u}_\varepsilon(t,\mathbf{x}) - \mathbf{div}\sigma_\varepsilon(t,\mathbf{x}) = 0 \qquad \forall(t,\mathbf{x}) \in (0,T)\times\Omega \tag{1}$$

with two initial conditions:

$$\mathbf{u}_\varepsilon(0,\mathbf{x}) = \mathbf{u}_0(\mathbf{x}/\varepsilon); \qquad \partial_t\mathbf{u}_\varepsilon(0,\mathbf{x}) = \mathbf{v}_0(\mathbf{x}/\varepsilon) \qquad \forall \mathbf{x} \in \Omega$$

where $\rho(\mathbf{x})$ is the density, and the stress σ and the deformation ϵ are defined by $\sigma_\varepsilon(t,\mathbf{x}) = \mathbf{C}(\mathbf{x})\epsilon_\varepsilon(t,\mathbf{x})$ and $\epsilon_\varepsilon(t,\mathbf{x}) = \frac{1}{2}(\nabla_{\mathbf{x}}\mathbf{u}_\varepsilon(t,\mathbf{x}) + \nabla^t_{\mathbf{x}}\mathbf{u}_\varepsilon(t,\mathbf{x}))$.

Here we assume that the fourth-order elasticity tensor of a randomly perturbed anisotropic medium satisfies:

$$\mathbf{C}(\mathbf{x}) = \mathbf{C}_0(\mathbf{x}) + \delta\mathbf{C}_0(\mathbf{x}) = \mathbf{C}_0(\mathbf{x})(1 + \sqrt{\varepsilon}\mathbf{C}_1(\mathbf{x}/\varepsilon))$$

where $\mathbf{C}_0$ is the elasticity tensor of the slowly varying background medium, and $\mathbf{C}_1$ is its fast fluctuations with amplitude $\sqrt{\varepsilon}$. The scale of variation of fluctuations is of order ε in order to ensure full interaction between propagating waves and random inhomogeneities; and the amplitude $\sqrt{\varepsilon}$ of fluctuations is chosen so that the energy can be significantly modified by the fluctuations in this order and also because too large fluctuations will lead to localization of wave energy. This fluctuation is modeled by a tensor-valued, statistically homogeneous mean zero random field $\mathbf{C}_1(\mathbf{y}), \mathbf{y} = \mathbf{x}/\varepsilon \in \mathbb{R}^3$.

2.2 Spatiotemporal Wigner measure of high-frequency elastic waves

For two fields $\mathbf{u}_\varepsilon(t,\mathbf{x})$ and $\mathbf{v}_\varepsilon(t,\mathbf{x})$, the spatiotemporal Wigner transform $\mathbf{W}_\varepsilon[\mathbf{u}_\varepsilon,\mathbf{v}_\varepsilon]$ is defined as:

$$\mathbf{W}_\varepsilon[\mathbf{u}_\varepsilon,\mathbf{v}_\varepsilon](t,\mathbf{x};\omega,\mathbf{k}) := \int_{\mathbb{R}^d} \mathbf{u}_\varepsilon(t-\frac{\varepsilon\tau}{2},\mathbf{x}-\frac{\varepsilon\mathbf{y}}{2}) \otimes \mathbf{v}^*_\varepsilon(t+\frac{\varepsilon\tau}{2},\mathbf{x}+\frac{\varepsilon\mathbf{y}}{2})e^{i(\tau\omega+\mathbf{y}\cdot\mathbf{k})}d\tau d\mathbf{y}$$

This definition generalizes the well-known temporal Wigner transform widely used in signal and images processing. Here it is properly scaled at ε^{-1} so as to contain all the fluctuations in this order.$\mathbf{W}_\varepsilon$ represents a distribution of energy density in time t and space $\mathbf{x}$ in terms of frequency ω and wave vector $\mathbf{k}$.

The Wigner measure, denoted by $\mathbf{W}$, is the weak limit of the Wigner transform $\mathbf{W}_\varepsilon$ as $\varepsilon \to 0$:

$$\mathbf{W}[\mathbf{u}_\varepsilon] := lim_{\varepsilon\to 0}\mathbf{W}_\varepsilon[\mathbf{u}_\varepsilon]$$

which can be interpreted as the energy density of waves in the phase space. The radiative transfer equation that we will derive is in terms of this quantity.

3 Radiative transfer equations

By developing a multi-scale asymptotic analysis of the wave equations (1) using spatiotemporal Wigner transforms, radiative transfer equations can by derived. They provide a good description of evolution of wave energy in the phase space in terms of the Wigner measure for high frequency waves in random media. We present hereafter main steps of the derivation of radiative transfer equations and more details can be found in relate literature [1, 2, 3].

Firstly, the following equations hold when the spatiotemporal Wigner transforms are applied to the wave equations (1):

$$\mathbf{W}_\varepsilon[\rho\partial_t^2\mathbf{u}_\varepsilon - \mathbf{div}\sigma_\varepsilon, \mathbf{u}_\varepsilon] = 0, \qquad \mathbf{W}_\varepsilon[\mathbf{u}_\varepsilon, \rho\partial_t^2\mathbf{u}_\varepsilon - \mathbf{div}\sigma_\varepsilon] = 0$$

then we use a two-scale asymptotic expansion of the Wigner transform as:

$$\mathbf{W}_\varepsilon(t,\mathbf{x},\mathbf{x}/\varepsilon;\omega,\mathbf{k}) = \mathbf{W}(t,\mathbf{x};\omega,\mathbf{k}) + \sqrt{\varepsilon}\mathbf{W}_1(t,\mathbf{x},\mathbf{x}/\varepsilon;\omega,\mathbf{k}) + \varepsilon\mathbf{W}_2(t,\mathbf{x},\mathbf{x}/\varepsilon;\omega,\mathbf{k}) + o(\varepsilon)$$

for these two equations and all the terms inside Wigner transforms are developed and expanded.

Parameter identification will be applied for first three orders $\mathrm{o}(\varepsilon^0), \mathrm{o}(\varepsilon^{\frac{1}{2}})$ and $\mathrm{o}(\varepsilon)$:

1) the order $\mathrm{o}(\varepsilon^0)$ gives the dispersion properties of $\mathbf{W}$ and also the spectral decomposition of Wigner measure:

$$\mathbf{W}[\mathbf{u}_\varepsilon] = \sum_\alpha \mathbf{p}_\alpha \mathbf{w}_\alpha[\mathbf{u}_\varepsilon]\mathbf{p}_\alpha{}^*$$

here $\mathbf{p}_\alpha$ is the eigenvector of Christoffel tensor;

2) the orders $o(\varepsilon^{\frac{1}{2}})$ and $o(\varepsilon)$ allow to derive the radiative transfer equations:

$$\begin{aligned}&\partial_t \mathbf{w}_\alpha^\pm(t,\mathbf{x};\omega,\mathbf{k}) \pm \left\{\omega_\alpha(\mathbf{x},\mathbf{k}), \mathbf{w}_\alpha^\pm(t,\mathbf{x};\omega,\mathbf{k})\right\} + \left[\mathbf{N}_\alpha(\mathbf{x},\mathbf{k}), \mathbf{w}_\alpha^\pm(t,\mathbf{x};\omega,\mathbf{k})\right] \\ &= \sum_{\beta=1}^{R} \int_{\omega_\alpha(\mathbf{k})=\omega_\beta(\mathbf{k}')} s_{\alpha\beta}(\mathbf{x},\mathbf{k},\mathbf{k}')[\mathbf{w}_\alpha^\pm(t,\mathbf{x};\omega,\mathbf{k}')] \frac{d\mathbf{k}'}{(2\pi)^3} - S_\alpha(\mathbf{x},\mathbf{k})\mathbf{w}_\alpha^\pm(t,\mathbf{x};\omega,\mathbf{k}) - \mathbf{w}_\alpha^\pm(t,\mathbf{x};\omega,\mathbf{k})S_\alpha^*(\mathbf{x},\mathbf{k})\end{aligned} \tag{2}$$

Here, the subscript α represents the different modes of waves (in isotropic media, one mode for P wave and two modes for S wave) and the superscript $\pm$ represent respectively the "forward" and the "backward" directions of waves; the energy density $\mathbf{w}_\alpha^\pm$ is the projection of the Wigner measure $\mathbf{W}$ for mode α in direction "+" or "-" and as a fonction of $(t,\mathbf{x};\omega,\mathbf{k})$; ω_α^2 is the eigen value of Christoffel tensor so $\omega_\alpha^2 = c_\alpha^2(x,k)|k|^2$ (c: wave velocity); the coupling matrix $\mathbf{N}_\alpha(\mathbf{x},\mathbf{k})$, related to the slow variations of the background, vanishes in homogeneous media and in 1D media; R is the number of different eigenvalues of the background medium; $s_\alpha(\mathbf{x},\mathbf{k},\mathbf{k}')$ is the differential scattering cross-section, namely the rate of conversion of energy with wave number $\mathbf{k}'$ into energy with wave number $\mathbf{k}'$ at $\mathbf{x}$ and $S_\alpha(\mathbf{x},\mathbf{k})$ is the total scattering cross-section.

In 2D isotropic media, the elasticity tensor $\mathbf{C}_0(\mathbf{x})$ are defined by two lamé's coefficients λ and μ, and the P and S waves modes are coupled in Eq.(2). The Wigner measure is expanded as: $\mathbf{W}[\mathbf{u}_\varepsilon] = w_P \mathbf{k}\otimes\mathbf{k} + w_S \mathbf{z}\otimes\mathbf{z}$, $\mathbf{z}\perp\mathbf{k}$. We give here the formula of the differential and total scattering cross-section :

$$\begin{aligned}
s_{PP}(\mathbf{k},\mathbf{k}')[w_P(\mathbf{k}')] &= \frac{\pi\,|\mathbf{k}|^2}{2\rho(\lambda+2\mu)}\left\{\lambda^2\hat{P}_{\lambda\lambda}(\mathbf{k}-\mathbf{k}') + 4\lambda\mu(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')^2\hat{P}_{\lambda\mu}(\mathbf{k}-\mathbf{k}') + 4\mu^2(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')^4\hat{P}_{\mu\mu}(\mathbf{k}-\mathbf{k}')\right\} w_P(\mathbf{k}') \\
s_{PS}(\mathbf{k},\mathbf{k}')[w_S(\mathbf{k}')] &= \frac{\pi\mathbf{c}_S^2\,|\mathbf{k}|^2}{2\rho}\left\{4(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')^4\hat{P}_{\mu\mu}(\mathbf{k}-\mathbf{k}')\right\} w_S(\mathbf{k}') \\
s_{SS}(\mathbf{k},\mathbf{k}')[w_S(\mathbf{k}')] &= \frac{\pi\mathbf{c}_S^2\,|\mathbf{k}|^2}{2\rho}\left\{(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')^4\hat{P}_{\mu\mu}(\mathbf{k}-\mathbf{k}')\right\} w_S(\mathbf{k}') \\
s_{SP}(\mathbf{k},\mathbf{k}')[w_P(\mathbf{k}')] &= \frac{\pi\mathbf{c}_S^2\,|\mathbf{k}|^2}{2\rho}\left\{4(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')^4\hat{P}_{\mu\mu}(\mathbf{k}-\mathbf{k}')\right\} w_P(\mathbf{k}') \\
S_\alpha(\mathbf{x},\mathbf{k}) &= \frac{1}{(2\pi)^2}\sum_\beta \int_{\omega_\alpha(\mathbf{k})=\omega_\beta(\mathbf{k}')} s_{\alpha\beta}(\mathbf{x},\mathbf{k},\mathbf{k}')d\mathbf{k}' \qquad (\alpha,\beta = P,S)
\end{aligned}$$

where $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ are unit wave number vectors, $\mathbf{c}_S$ is velocity of S wave, $\hat{P}$ is the power spectral density function of the fast fluctuations of corresponding coefficients. This implies that the variations of $\mathbf{C}_1$ contribute only the right-hand side of radiative transfer equation, namely the scattering of waves by inhomogeneities at fast scale.

4 Energy based residual error analysis in 1D case

In this section, we apply a posteriori residual error analysis to the radiative transfer equation. In general, we do not solve Eq.(2) and it is only used for evaluating the numerical solutions of Eq.(1). The Wigner transform of these solutions is calculated and projected into Eq.(2) in order to find the residuals. So this is a posteriori error analysis of Eq.(1) but in terms of energy quantity which satisfies Eq.(2).

In 1D heterogeneous case, Eq.(2) can be simplified as (here only the direction "+" is considered):

$$\begin{aligned}\partial_t \mathrm{W}(t,x;\omega,k) + c_0(x)\partial_x \mathrm{W}(t,x;\omega,k) - {c_0}'(x)\partial_k \mathrm{W}(t,x;\omega,k) \\ = \frac{c_0(x)k^2}{4}\hat{P}(2k)\left\{\mathrm{W}(t,x;\omega,-k) - \mathrm{W}(t,x;\omega,k)\right\}\end{aligned}$$

where wave velocity $c_0 := \sqrt{E/\rho}$, E : Young's modulus, and $E = E_0(1+\sqrt{\varepsilon}E_1)$.

We can denote $\mathrm{T} := \partial_t\mathrm{W} + c_0\partial_x\mathrm{W}$ for transport part of radiative transfer equation and $\mathrm{S} := \frac{c_0k^2}{4}\hat{P}(2k)\left\{\mathrm{W}(-k) - \mathrm{W}(k)\right\}$ for its scattering part. We assume $u_{h,\Delta t}$ the finite element solutions. h is the mesh size and Δt is the time step. Then the residual errors are defined by :

$$\begin{aligned}\mathrm{R}[u_{h,\Delta t}] :=& \mathrm{T}[u_{h,\Delta t}] - \mathrm{S}[u_{h,\Delta t}] \\ =& \partial_t \mathrm{W}[u_{h,\Delta t}] + c_0 \partial_x \mathrm{W}[u_{h,\Delta t}] - {c_0}' \partial_k \mathrm{W}[u_{h,\Delta t}] - \frac{c_0 k^2}{4} \hat{P}(2k) \left\{ \mathrm{W}[u_{h,\Delta t}](-k) - \mathrm{W}[u_{h,\Delta t}](k) \right\}\end{aligned} \tag{3}$$

It is worth to note that in homogeneous case, the right-hand side of Eq.(3) equals to zero, so the following transport equation is obtained:

$$\partial_t \mathrm{W} + c_0 \partial_x \mathrm{W} = 0$$

By using the properties of homogeneous pseudo-differential operator $\varphi(k)$ in space, defined by $\varphi(\varepsilon D_x) u(x) := \int e^{ikx} \varphi(\varepsilon k) \hat{u}(k) dk$:

$$\mathrm{W}_\varepsilon[\varphi(\varepsilon D_x) u_\varepsilon, u_\varepsilon] = \varphi(k + \frac{\varepsilon D_x}{2}) \mathrm{W}_\varepsilon[u_\varepsilon]$$

$$\mathrm{W}_\varepsilon[u_\varepsilon, \varphi(\varepsilon D_x) u_\varepsilon] = \mathrm{W}_\varepsilon[u_\varepsilon] \varphi^*(k - \frac{\varepsilon D_x}{2})$$

Taking $\varphi(\varepsilon D_x) = E \varepsilon D_x$, we can prove: $\mathrm{W}_\varepsilon[E \partial_x u_\varepsilon, u_\varepsilon] = 2\mathrm{Re}\left\{\mathrm{W}_\varepsilon[u_\varepsilon, \sigma_\varepsilon]\right\}$. The same idea can be applied in time: $\mathrm{W}_\varepsilon[\partial_t u_\varepsilon, u_\varepsilon] = 2\mathrm{Re}\left\{\mathrm{W}_\varepsilon[u_\varepsilon, v_\varepsilon]\right\}$.

We obtain finally in this particular case the following residual errors where only the transport term exists:

$$\mathrm{R}[u_{h,\Delta t}] = 2\mathrm{Re}\left\{\mathrm{W}[u_{h,\Delta t}, v_{h,\Delta t}]\right\} + \frac{2c_0}{E} \mathrm{Re}\left\{\mathrm{W}[u_{h,\Delta t}, \sigma_{h,\Delta t}]\right\} \tag{4}$$

5 Numeric examples

In this section, we will introduce the numerical calculations of Wigner transform in 1D and 2D media, then the residual errors defined in Eq.(4) and Eq.(3) are respectively calculated in 1D homogeneous case and heterogeneous case.

5.1 Wigner transform in 1D and 2D media

We consider here wave propagation in 1D homogeneous elastic bar. A force whose evolution in time is a Ricker wavelet is loaded in one end and another is free of charge. Principal parameters are given here: $\omega_{max} = 8.31\text{e}5\text{rad/s}$ (maximum frequency of Ricker), $L = 1\text{m}$ (length of bar), $E = 7\text{e}10\text{Pa}$, $\rho = 2500\text{kg/m}^3$. The numerical finite element solutions are solved by time discontinuous space-time Galerkin method with mesh sizes $(\lambda(\omega_{max})/h = 20)$ and $\Delta t = h/c_0$.

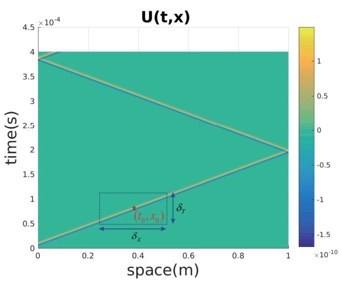


Figure 1: $u(t,x)$

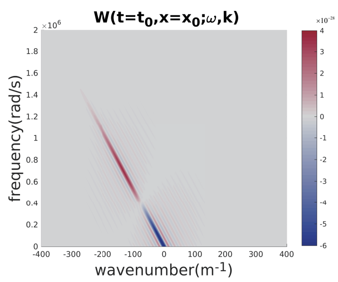


Figure 2: $\mathrm{W}(t_0, x_0; \omega, k)$ 1D

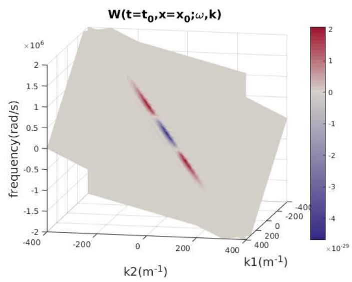


Figure 3: $\mathrm{W}(t_0, x_0; \omega, k)$ 2D

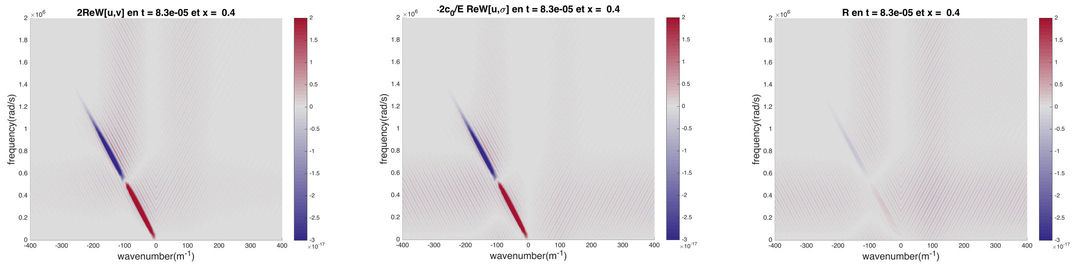
Fig.(1) gives the displacement field $u(t,x)$ in space time and Fig.(2) is the spatiotemporal Wigner transform of $u(t,x)$ for one point (t_0, x_0) in wave front, where $\hat{\mathbf{k}} = (1,0,0)$. The calculation area defined by (δ_t, δ_x) in Fig.(1) is well chosen so that the Wigner transform can present the energy distributions clearly.

We give also an example for spatiotemporal Wigner transform of wave propagation with $\hat{\mathbf{k}} = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, 0)$ in 2D homogeneous isotropic plate in Fig.(3). We can find that in these two figures wave energy is located along relation of dispersion of waves in spectral domain.

5.2 Residuals in homogeneous media

The model defined in section 5.1 is used also here for residuals, and the numerical solutions are calculated with different mesh sizes ($\lambda(\omega_{max})/h = 2, 4, 10, 20$). Then in each case, we can obtain the Wigner transform $\mathrm{W}(t, x; \omega, k)$ for all points of a grid in space-time domain.

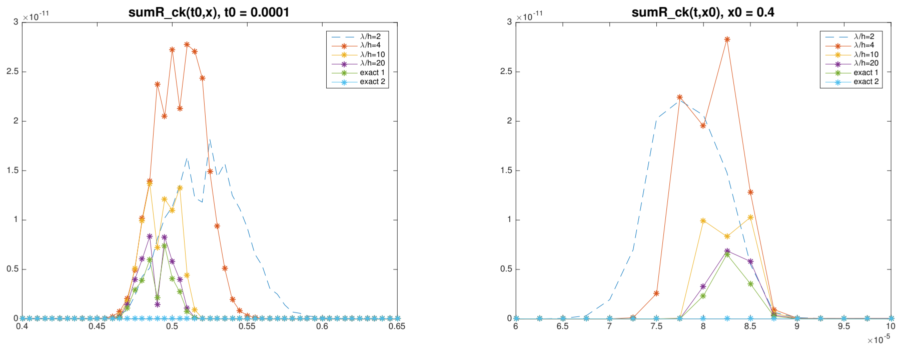
Then Eq.(4) is calculated and illustrated in Fig.(4) for only one point (t_0, x_0) here. We observe that residuals errors are mainly located along the characteristic line $\omega = \mp ck$. Some noticeable fluctuations are also found around axis caused by leakage of frequency since we have to do Matlab FFT in limited area. Several solutions have been proposed by researchers to overcome these edge effects [4] but in general case, we can not find any method to remove totally these errors.



(a) $2\mathrm{Re}\{\mathrm{W}[u, v]\}$ (b) $-\frac{2c_0}{E}\mathrm{Re}\{\mathrm{W}[u, \sigma]\}$ (c) R

Figure 4: Residuals for $\lambda/h = 4$ in homogeneous media

So in order to evaluate errors more reasonably, we define $\tilde{\mathrm{R}}(t, x) := \int |\mathrm{R}(t, x; \omega, k)|\, d\omega dk$ and the integral area is only around $\omega = \mp ck$. Its width is carefully chosen as $2\Delta k$ (Δk is frequency resolution) so that it contains well the real residual errors but not too much fluctuations.



(a) $\tilde{R}(t_0, x)$ (b) $\tilde{R}(t, x_0)$

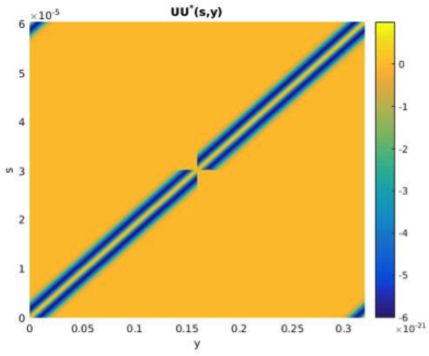
Figure 5: $\tilde{R}(t, x)$ at a certain moment or position

Finally, the residual errors in all time-space area is obtained for different mesh size. In Fig.(5) we observe the tendency of decreasing of errors with increasing of number of elements per wavelength as we expected ($\lambda/h = 2$ can be neglected). We give two different results of exact solutions with different interpolation in space-time. In fact, the second one is interpolated exactly with respect to $h = c_0\Delta t$ and in this particular case, we can correct the discontinuities across the border of calculating area, see Fig.(6), which allows us to eliminate largely the edge effects. So the errors in second case are much smaller in Fig.(5).

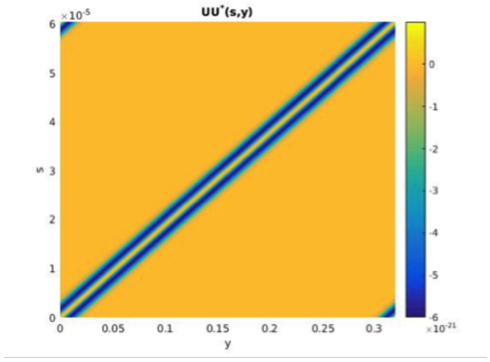
5.3 Residuals in heterogeneous media

The same calculations can be applied in 1D heterogeneous case, where random fields E around E_0(assumed to be constant) in Fig.(7) are generated by its power spectral density function $\hat{P}(k)$, defined by Fig.(8).

In Fig.(9) we just give first results of $\mathrm{T}, \mathrm{S}, \mathrm{R}$ with $\lambda/h = 20$ with removing roughly the fluctuations by FFT and the cross terms of Wigner transform. We notice that the scattering



(a) uu^*



(b) uu^* corrected

Figure 6: Correction of discontinuities of FFT in one period

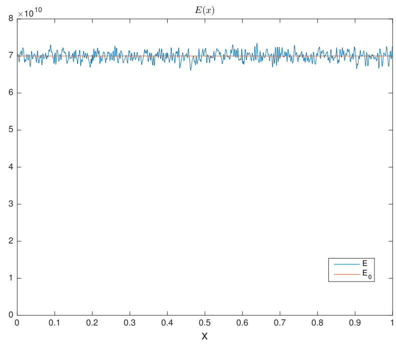


Figure 7: $E(x)$

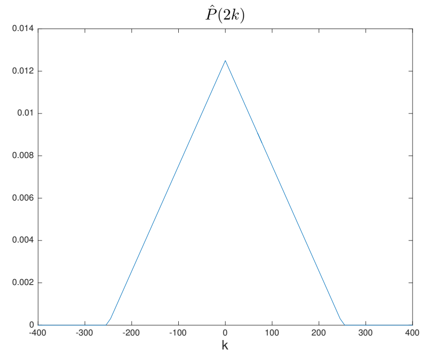
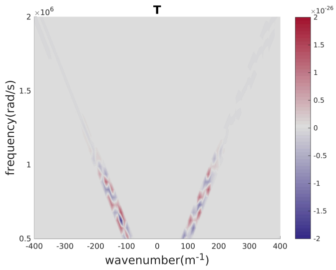
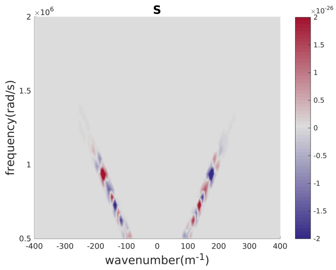


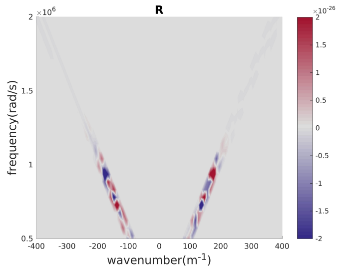
Figure 8: $\hat{P}(2k)$



(a) T



(b) S



(c) R

Figure 9: Residuals for $\lambda/h = 20$ in heterogeneous media

part is large and very different with the transport part. Since the mesh is relatively fine here, it is expected that these two terms should be approximatively equal. So these results are currently being improved, and the influence by numerical interference should be carefully considered.

6 Conclusion

In conclusion, we have proposed a new error analysis method based on radiative transfer equation in terms of energy quantity: the radiative transfer equation is derived in different media and numerical tools for calculating Wigner transforms in 1D and 2D have been developed and validated; then associated residual errors are defined and developed for transport equation.Temporarily the numerical results in 1D homogenous case validate our method but the heterogeneous case still need to be improved. The current work concerns high dimensional heterogeneous cases.

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