Modeling Elastic Waves in Heterogeneous Anisotropic Media using a k-Space Method

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***Abstract*—We generalize the theory of the k-space method to the case of elastic wave propagation in heterogeneous anisotropic media. The k-space operator is derived in the spatially continuous form using the displacement formalism of elastodynamics. The k-space scheme is then discretized in space using a Fourier collocation spectral method. This leads to an efficient and accurate numerical algorithm, where the time advancement can be performed in order of N operations, where N is the number of unknowns. As opposed to the classical k-space theory for the elastic waves in isotropic media [1], [2], the new algorithm does not need any field splitting. Hence, it is more efficient once used to model isotropy. The proposed method is temporally exact for homogeneous media, unconditionally stable for heterogeneous media, and also allows larger time-steps without loss of accuracy. We validate the method against canonical model problems of elastodynamics.**

Keywords: k-space method; elastic waves; heterogeneous media; anisotropy; Fourier collocation spectral method; pseudospectral method; explicit time integration

I. Introduction

Elastic wave propagation in inhomogeneous anisotropic media has widespread applications in many different areas of science and technology. Therefore, efficient and accurate numerical methods are of great importance. The dominant conventional methods such as finite elements or finite-differences with the standard time integration schemes are cumbersome and slow as they require many points per wavelength (PPW) for a satisfactory accuracy. They may also exhibit a poor performance for problems in heterogeneous media. Spectral methods are excellent alternatives for the spatial discretization as they can dramatically relax the PPW requirement. For time integration, explicit schemes are strongly preferred over implicit ones, as spectral methods produce dense matrices which make implicit schemes costly. However, the classical explicit schemes are generally conditionally stable and sensitive to dispersion errors. We present a k-space pseudospectral method which (1) uses a spectral discretization technique, (2) introduces an integration scheme that is explicit and unconditionally stable and can be parameterized to minimize the dispersion error, (3) can be efficiently implemented using the fast Fourier transform algorithm, and (4) handles propagation in heterogeneous media very efficiently. In this paper, the main properties of the method are explained, however, the proofs are not given for the sake of brevity.

In this study, the following notations are adopted: i, j, k represent the spatial dimensions. I, J, K indicate the collocation grid points associated with the discretized domain. $(\cdot)_i$ and $(\cdot)_{ij}$ indicate the components of the vector and tensor fields whereas $(\cdot)_{,i}$ and $(\cdot)_{,ij}$ represent the partial derivatives in Euclidean coordinates. Throughout this paper, the summation convention is used for i, j, k unless otherwise specified. If an index is represented in parentheses, i.e., $(\cdot)_{(i)}$, it is counted as a free index (i.e., no summation over this index). $\otimes$ represents the dyadic product. tr indicates the trace operator. i represents the imaginary number (i.e., $\mathrm{i} = \sqrt{-1}$). $(\cdot)\big|_{(\cdot)}$ indicates restriction of a variable to a point.

II. Governing equations

Wave propagation in general d-dimensional linear anisotropic elastic media is governed by the linearized momentum balance law and a linear constitutive relation between the stress and strain. The governing equations are as follows.

$$\rho \ddot{u}_i = \sigma_{ij,j} + f_i, \tag{1a}$$

$$\sigma_{ij} = C_{ijkl} u_{(k,l)}, \tag{1b}$$

$$u_{(k,l)} = \frac{1}{2}(u_{k,l} + u_{l,k}), \tag{1c}$$

in $\mathbb{R}^d \times (0, T]$, with u and σ being the displacement and stress fields, respectively. The radiation condition is specified as $\|x\|_2 \to \infty$, with $x = (x_1, \ldots, x_d)$. The initial conditions are given as

$$u_i(x, 0) = \varphi_i(x),\ \dot{u}_i(x, 0) = \psi_i(x),\ \text{in } \mathbb{R}^d. \tag{2}$$

C is the fourth-order elasticity tensor with the major and minor symmetries, i.e., $C_{ijkl} = C_{klij}$ and $C_{ijkl} = C_{jikl} = C_{ijlk}$. We also assume that C is positive definite.

II. Construction of the k-space operator

Consider a homogeneous medium (i.e., the elasticity tensor C and the density ρ are spatially uniform). Using the symmetry of C, equations (1a), (1b), and (1c) can be combined to write the one-field displacement formalism as

$$\rho \ddot{u}_i = C_{ijkl} u_{k,lj} + f_i,\ \text{in } \mathbb{R}^d \times (0, T], \tag{3a}$$

$$u_i(x, t = 0) = \varphi_i(x),\ \text{in } \mathbb{R}^d, \tag{3b}$$

$$\dot{u}_i(x, t = 0) = \psi_i(x),\ \text{in } \mathbb{R}^d. \tag{3c}$$

Consider $w \in L^2(\mathbb{R}^d)$, we write the Fourier transform and its inverse as

$$\hat{w}(\xi) = (\mathcal{F}_{x\to\xi} w)(\xi) = \int_{\mathbb{R}^d} w e^{-\mathrm{i}\xi\cdot x} dx, \tag{4a}$$

$$w(x) = (\mathcal{F}^{-1}_{\xi\to x}\hat{w})(x) = (2\pi)^{-d}\int_{\mathbb{R}^d} \hat{w} e^{\mathrm{i}\xi\cdot x} d\xi, \tag{4b}$$

and recall the differentiation property in the Fourier space that is $\mathcal{F}_{x\to\xi} w_{,j} = i\xi_j \hat{w}$. $\mathcal{F}$,$\mathcal{F}^{-1}$ represent the Fourier and the inverse Fourier transforms, respectively. Equation (3) in the Fourier space is given as

$$\rho\ddot{\hat{u}}_i + \xi_j C_{ijkl}\xi_l \hat{u}_k = \hat{f}_i, \tag{5}$$

with

$$\hat{u}_i(\xi, 0) = \hat{\varphi}_i(\xi),\ \dot{\hat{u}}_i(\xi, 0) = \hat{\psi}_i(\xi). \tag{6}$$

Let $\Gamma = 1/\rho\xi\cdot C\cdot\xi$. It is then easy to check that Γ is symmetric positive definite. Equation (5) is now a system of ordinary differential equations coupled in terms of the components of the wave number vector ξ. We proceed with integrating this system exactly. For this, we shall henceforth drop the body source term and proceed with the homogeneous equation. This is by use of the *Duhamel* principle.

Since Γ is symmetric positive definite, it has a unique spectral decomposition of the form $\Gamma = \sum_{i=1}^d \lambda_i^2 N_i \otimes N_i$, where λ_i^2's are the eigenvalues and N_i's are the eigenvectors of Γ, with $N_i\cdot N_j = \delta_{ij}$. We may alternatively write this as $\Gamma = Q\Lambda Q^T$, where Q is an orthogonal tensor (i.e., $Q^{-1} = Q^T$, with Q^T indicating the transpose of Q) whose columns are N_i's. Λ is a diagonal tensor with λ_i^2's being the entries. Define $\hat{\vartheta}_i = Q_{ij}\hat{u}_j$, we can then rewrite equation (5) as

$$\ddot{\hat{\vartheta}}_i + \lambda_{(i)}^2 \hat{\vartheta}_i = 0, \tag{7}$$

with

$$\hat{\vartheta}_i(\xi, 0) = Q_{ij}\hat{\varphi}_j(\xi),\ \dot{\hat{\vartheta}}_i(\xi, 0) = Q_{ij}\hat{\psi}_j(\xi). \tag{8}$$

This is now a system of uncoupled equations for each ξ, each of which with a general solution $\hat{\vartheta}_i(\xi, t) = A\cos(\lambda_i t) + B\sin(\lambda_i t)$. Enforcing the initial conditions, we get

$$\hat{\vartheta}_i(\xi, t) = Q_{ij}\hat{\varphi}_j(\xi)\cos(\lambda_{(i)} t) + \frac{Q_{ij}\hat{\psi}_j(\xi)}{\lambda_{(i)}}\sin(\lambda_{(i)} t). \tag{9}$$

Next, we proceed with the numerical integration of equation (5) using some standard scheme. This is the base strategy for constructing the k-space integrator [1], [2]. We focus our construction on the standard leapfrog scheme as a well-established explicit scheme for wave problems. This leads to

$$\frac{\hat{\vartheta}_i^{(n+1)} - 2\hat{\vartheta}_i^{(n)} + \hat{\vartheta}_i^{(n-1)}}{\Delta t^2} = \lambda_{(i)}^2 \hat{\vartheta}_i^{(n)},\ \Delta t = t^{n+1} - t^n. \tag{10}$$

It would be useful to introduce a more compact notation. Define the following linear forward and backward differencing operators.

$$\bar{\partial} u_i^n := \frac{u_i^{(n)} - u_i^{(n-1)}}{\Delta t},\ \partial u_i^n := \frac{u_i^{(n+1)} - u_i^{(n)}}{\Delta t}. \tag{11a}$$

Equation (10) can now be expressed as

$$\partial\bar{\partial}\hat{\vartheta}_i^{(n)} = \lambda_{(i)}^2 \hat{\vartheta}_i^{(n)}. \tag{12}$$

Next, we construct the leapfrog stencil using the exact solution, which by using the trigonometric identities can be written as

$$\partial\bar{\partial}\hat{\vartheta}_i^{(n)} = -\lambda_{(i)}^2 \operatorname{sinc}^2(\lambda_{(i)}\Delta t/2)\hat{\vartheta}_i^{(n)}, \tag{13}$$

where $\operatorname{sinc}(\cdot) = \sin(\cdot)/(\cdot)$. Note that the summation convection *is not* used in equations (12) and (13). We rewrite equation (13) in the invariant form for simplicity as

$$\partial\bar{\partial}\hat{\Theta}^{(n)} = \tilde{\Lambda}\hat{\Theta}^{(n)}, \tag{14}$$

where $\Theta = (\vartheta_1, \dots, \vartheta_d)$ and $\tilde{\Lambda}_{ij} = -\lambda_{(i)}^2 \operatorname{sinc}^2(\lambda_{(i)}\Delta t/2)\delta_{ij}$. Note $\Theta = Qu$. Replacing this in equation (14) and using the orthogonality of Q, we construct the exact time integration in terms of u as

$$\partial\bar{\partial}\hat{u}^{(n)} = \tilde{\Gamma}\hat{u}^{(n)}. \tag{15}$$

where $\tilde{\Gamma} = -Q\tilde{\Lambda}Q^T = -\sum_{i=1}^d \tilde{\lambda}_i^2 N_i \otimes N_i$, $\tilde{\lambda}_{(i)}^2 := \lambda_{(i)}^2 \operatorname{sinc}^2(\lambda_{(i)}\Delta t/2)$. We use this to define the k-space operator as follows.

Definition II.1. k-space operator. $\mathcal{M} : [L^2(\mathbb{R}^d)]^d \to [L^2(\mathbb{R}^d)]^d$ *is the k-space operator defined with the following kernel.*

$$\mathcal{M} := (2\pi)^{-d}\int_{\mathbb{R}^d\times\mathbb{R}^d} \tilde{\Gamma}(\xi) e^{\mathrm{i}\xi\cdot(x-y)} dy d\xi. \tag{16}$$

Using this definition, equation (15) is written as

$$\partial\bar{\partial} u^{(n)} = \mathcal{M} u^{(n)}, \tag{17}$$

Note that equation (17) is *exact* for the model problem equation (3).

III. Heterogeneous media and the k-space derivative

When the medium is heterogeneous, the elasticity tensor C and the density ρ vary spatially. So, the problem is governed by the following system of equations.

$$\ddot{u}_i(x, t) = \frac{1}{\rho(x)}(C_{ijkl}(x) u_{(k,l)})_{,j} + f_i(x, t). \tag{18}$$

In such a case, the direct application of the Fourier technique results in global coupling of the equations (which is a consequence of changing multiplication to convolution). This involves a kernel that typically requires $\mathcal{O}(N^3 - N^4)$ operations when discretized. In this section, we attempt to construct an accurate and efficient time integrator, which along with a collocation Fourier spectral discretization, will bring down the cost of computation to $\mathcal{O}(N\log(N))$.

For this we proceed with integrating the so-called stress-velocity formalism, which can be achieved by re-arranging the time derivatives over the constitutive equation and the conservation of momentum. This can be written as

$$\rho\dot{v}_i = \sigma_{ij,j} + f_i, \tag{19a}$$
$$\dot{\sigma}_{ij} = C_{ijkl}v_{(k,l)}. \tag{19b}$$

Introducing a time-staggered leapfrog scheme, it is then possible to write equation (19) in a predictor-corrector form of

$$\bar{\partial}v_i^{n+1/2} = \frac{1}{\rho}\sigma_{ij,j}^n + \frac{1}{\rho}f_i^n, \tag{20a}$$
$$\bar{\partial}\sigma_{ij}^{n+1} = C_{ijkl}v_{(k,l)}^{n+1/2}. \tag{20b}$$

Proposition III.1. *The predictor-corrector form of equation (20) and the leapfrog scheme are equivalent.*

Application of the k-space method to the case of the non-constant coefficients model can be motivated by noting

$$\partial_j = \mathrm{Id}\,\partial_j\,\mathrm{Id} = \mathcal{F}^{-1}\mathcal{F}\partial_j\mathcal{F}^{-1}\mathcal{F} = \mathcal{F}^{-1}\mathrm{i}\xi_j\mathcal{F},$$

so that for a function $w(x)$

$$\partial_k w(x) = \mathcal{F}^{-1}\mathrm{i}\xi_k\mathcal{F}w(x),$$
$$\partial_i w(x)\partial_j = \mathcal{F}^{-1}\mathrm{i}\xi_i\mathcal{F}w(x)\mathcal{F}^{-1}\mathrm{i}\xi_j\mathcal{F}.$$

This motivates to introduce a modification to the wave number vector using the k-space operator such that the numerical scheme becomes exact for homogeneous media. This leads to the k-space derivative defined as below.

Definition III.2. k-space derivative. *Consider a model homogeneous medium with the elasticity tensor $\bar{C}$, density $\bar{\rho}$, and $\Gamma = 1/\bar{\rho}\xi\cdot\bar{C}\cdot\xi$. Let $\Gamma = \sum_{i=1}^d \bar{\lambda}_i^2\bar{N}_i\otimes\bar{N}_i$ be the spectral decomposition of Γ. Then for $w(x)\in L^2(\mathbb{R}^d)$, the k-space derivative $D_j : L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)$ is defined as*

$$(D_j w)(x) = (2\pi)^{-d}\int_{\mathbb{R}^d\times\mathbb{R}^d} i\tilde{\xi}_j(\xi)w(y)e^{i\xi\cdot(x-y)}dyd\xi, \tag{21}$$

where

$$\tilde{\xi} := \Xi(\xi)\cdot\xi,\ \Xi(\xi) := \sum_{i=1}^d \mathrm{sinc}(\bar{\lambda}_i\Delta t/2)\bar{N}_i\otimes\bar{N}_i.$$

We shall now construct the k-space scheme by replacing the derivatives in equation (20) by the k-space derivative. This becomes

$$\bar{\partial}v^{n+1/2} = \frac{1}{\rho}\,\mathrm{tr}(D\otimes\sigma^n) + \frac{1}{\rho}f^n, \tag{22a}$$
$$\bar{\partial}\sigma^{n+1} = C : D^s\otimes v^{n+1/2}, \tag{22b}$$

where D^s is the symmetric k-space gradient, i.e.,

$$D^s\otimes v = \frac{1}{2}\Big(D\otimes v + (D\otimes v)^T\Big).$$

Proposition III.3. *The k-space scheme is exact for homogeneous media.*

For heterogeneous media, the model homogeneous problem is chosen to achieve certain properties such as improved stability or accuracy. A convenient choice is given as below.

Theorem III.4. *The k-space scheme is unconditionally stable for heterogeneous media if*

$$\bar{\lambda}_i(\xi) = \sup_{x\in\mathbb{R}^d}\lambda_i(x,\xi),\ \bar{N}_i = N_i(\bar{\lambda}_{(i)}).$$

IV. Spectral spatial discretization

In the previous sections, only time discretization was introduced. A convenient and efficient choice for the spatial discretization of the k-space scheme, equation (22), is the collocation spectral method. Spectral methods are in general efficient and accurate numerical algorithms with widespread applications in computational science. Efficiency follows from the fact that typically they can be implemented using fast algorithms such as the fast Fourier transform (FFT). They are spectrally accurate since they construct the approximate solution using a spectral basis. Among these, *collocation* methods are suitable candidates for non-constant coefficients problems [3], such as the case of interest in this paper. Here, we consider a Fourier based collocation method to spatially discretize the k-space scheme.

Let $V_i, T_{ij}\in l^2(\mathbb{W})$ be the approximations to v_i, σ_{ij}, i.e., $V_{iI}^n \approx v(X^I, t^n)$, $T_{ijI}^n \approx \sigma_{ij}(X^I, t^n)$, where $\mathbb{W}\in\mathbb{Z}^d$ is the d-dimensional periodic lattice. $(\cdot)_I$ or $(\cdot)|_I$ denote the field at the collocation grid points X^I. The collocation expansions are given as $V_{iI} = \sum_K \hat{V}_i\phi_K(X^I)$, $T_{ijI} = \sum_K \hat{T}_{ij}\phi_K(X^I)$, with $\phi_K(X^I) = e^{\mathrm{i}K\cdot X^I}$, the Fourier basis function, and $K, I\in\mathbb{W}$. $X^I = (2\pi I_1/L_1,\cdots,2\pi I_d/L_d)$, where L_i is the size of the lattice along x_i. The k-space collocation scheme is then written as

$$\bar{\partial}V^{n+1/2}\Big|_I = \frac{1}{\rho}\,\mathrm{tr}(\mathbb{D}\otimes T^n)\Big|_I + \frac{1}{\rho}F_I^n, \tag{23a}$$
$$\bar{\partial}T^{n+1}\Big|_I = C : \mathbb{D}^s\otimes V^{n+1/2}\Big|_I, \tag{23b}$$

where $F_I^n = f(X^I, t^n)$ and $\mathbb{D}$ denotes the discrete k-space derivative operator defined as below.

Definition IV.1. Discrete k-space derivative. *Consider $U\in l^2(\mathbb{W})$, the discrete k-space derivative is defined as*

$$\mathbb{D}_j U\Big|_I := \sum_{K\in\mathbb{W}}\tilde{K}_j(K)\hat{U}(K)e^{iK\cdot X^I}, \tag{24a}$$
$$\hat{U}(K) = |\mathbb{W}|^{-1}\sum_{I\in\mathbb{W}}U(X^I)e^{-iK\cdot X^I}, \tag{24b}$$

and the discrete symbol is given as

$$\tilde{K}_i(K) := i\Xi_{ij}(K)K_j. \tag{25}$$

Remark The discrete k-space derivative can be evaluated by means of the discrete Fourier transform (DFT). This further allows application of the fast Fourier transform (FFT), hence makes the computation very efficient.

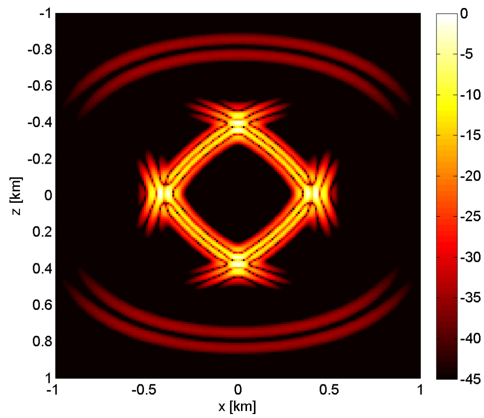

Fig. 1: Snapshot of the absolute value of the displacement field in a homogeneous three-dimensional transversely isotropic medium on the (y, z) plane at $x = 0$. The colormap is in the dB scale. Various wavetypes are in excellent agreement with the analytical ones [4], [5].

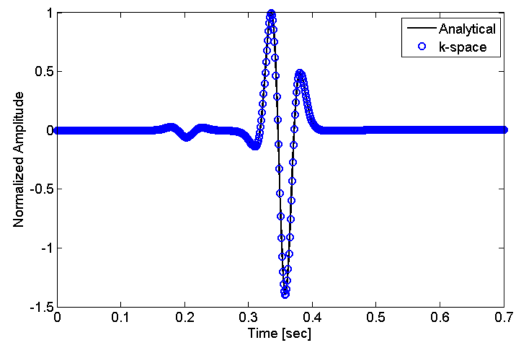

Fig. 2: The displacement profile along the axis of symmetry as a function time at $728.9\,\mathrm{m}$ away from the source in a homogeneous three-dimensional transversely isotropic medium. Analytical solution (solid), k-space solution (circles).

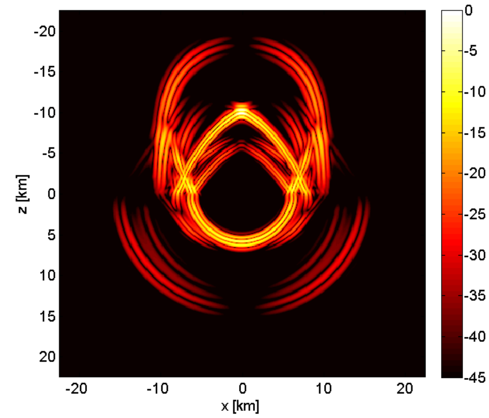

Fig. 3: Snapshot of the absolute value of the velocity field in the two-dimensional joint half-space problem. The colormap is in the dB scale. Various wavetypes are in excellent agreement with the ones of the previous studies [5], [6].

V. Examples

A. A quantitative assessment: A point disturbance in a three-dimensional homogeneous transversely isotropic media

As the first examples, consider a point force source pulsating in an infinite homogeneous transversely isotropic media made of *zinc*. The analytical solution to this problem is given in [4]. We use the simulation setting of [5]. The input waveform is a Ricker wavelet with the frequency of $170\,\mathrm{kHz}$ and time delay of $6\,\mu\mathrm{s}$. A snapshot of the displacement vector field is shown in Fig. 1. The time profile of the arrived wavefronts at $728.9\,\mathrm{m}$ from the source is shown side by the side the analytical solution in Fig. 2. The simulation was run with a CFL number where the standard leapfrog scheme is unstable. As can be seen the k-space solution is stable and has allowed a larger choice of time-step without loss of accuracy.

B. A qualitative assessment: Wave propagation in two-dimensional joint half-spaces

Closed form analytical solutions for heterogeneous anisotropic media do not generally exist. We provide a qualitative evaluation of the wave propagation in joint halfspaces made of *zinc* and the isotropic version of *zinc*. This problem has been studied by [5], [6]. The problem configuration is given in [5]. A snapshot of propagation at the time the waveforms are well developed are shown in Fig. 3. The wavefronts are in agreement with the ones reported by [5], [6].

VI. Summary

We have developed a k-space method to model elastic wave propagation in heterogeneous anisotropic media. The k-space method is *explicit* and *unconditionally stable*. The method was carefully designed to achieve a high level of efficiency and accuracy. The former is by virtue of the FFT-based implementation of the method, where $\mathcal{O}(N \log(N))$ operations are required at each time-step to advance the solution. Furthermore, the k-space operator was derived from the displacement formalism, which led to an algorithm without field splitting as oppose to the conventional k-space techniques.

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