

Forward Scattering Series and Padé Approximants for Acoustic Wavefield Propagation in a Vertically Varying Medium

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Abstract. We present the application of the theory of Padé approximants to extending the perturbative solutions of acoustic wave equation for a three dimensional vertically varying medium with one interface. These type of solutions have limited convergence properties depending on either the degree of contrast between the actual and the reference medium or the angle of incidence of a plane wave component. We show that the sequence of Padé approximants to the partial sums in the forward scattering series for the 3D wave equation is convergent for any contrast and any incidence angle. This allows the construction of any reflected waves including phase-shifted post-critical plane waves and, for a point-source problem, refracted events or headwaves, and it also provides interesting interpretations of these solutions in the scattering theory formalism.

AMS subject classifications: 35P25, 35J05, 34E10

Key words: Acoustic wave modeling, forward scattering series, Padé approximants.

1 Introduction

Many fields of non-destructive evaluation of a medium properties involve an acoustic, elastic or electro-magnetic experiment in which a natural or artificially created wave propagates through that medium and is recorded outside of the medium. The goal in such an experiment is to process the recorded wave, the data, to determine the medium's internal structure (imaging) and properties (inversion). Examples of such fields of applications are geophysical exploration for natural resources, medical imaging, remote sensing in engineering, whole earth seismology, astronomy, military radar and underground object detection, etc. Their tremendous economical, social and military importance is evident.

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In order to extract meaningful and useful information from the recorded wave-field, one needs to predict or model how the wave-field propagates in different types of complex settings. Ideally, one would be able to solve exactly the differential equations describing the propagation of the wave-field and add boundary conditions to describe different structures embedded in that medium. The solutions of such a boundary value problem would characterize the wave propagation through the medium, and its interactions with the complex structures it encounters, and would construct the wave-field everywhere inside and outside the medium. Unfortunately, such exact analytical solutions are difficult (and most often impossible) to obtain. This led to the development of alternative methods, for example numerical, for modeling the propagation of the wave-field in complex realistic settings; from these we mention least squares [12], finite differences [2,3,21], ray tracing [8], Fourier or pseudo-spectral methods [26], finite elements [9], reflectivity [15] and [31] as well as other hybrid methods [14]. A compilation of classical papers describing the finite differences and finite element methods in geophysics, their accuracy and different types of boundary conditions appeared in [22].

Many other methods, either new or derived from these ones, have been developed and implemented, each one trying to address a specific issue or downside in the methods listed above. For example the modeling techniques based on Kirchhoff integral [16], $f-k$ solutions to the wave equation [39], paraxial extrapolators method [10], Gaussian beam methods [24,25], hyperbolic superposition [27], scattering theory [42], lattice Boltzmann method [17] just to mention a few of them. All these methods have different assumptions, strengths and limitations. One feature shared by all the modeling methods, is that, as the complexity of the geological models increases, the computational requirements also increase to very expensive, and sometimes prohibited, values. Often a lower and cheaper alternative is chosen to model the wave-field in the detriment of accuracy. New methods and alternatives are sought and developed every year (see e.g. the Seismic Modeling sections at the American Geophysical Union (AGU) and Society for Exploration Geophysicists (SEG) annual meetings) to address some of the difficulties, execution time and computational costs in modeling wave-field propagation in complex sub-surface conditions.

In this paper we discuss a recently developed tool, for modeling the propagation of seismic wavefields, based on the scattering theory, the forward scattering series. Scattering theory is a powerful and useful method for analyzing wave propagation in a given medium (see e.g. [32,42]). As any form of perturbation theory, it relates the propagation of the wave in that medium with the propagation of the wave in a reference medium and a perturbation operator which describes the difference between the two media. The forward problem is to construct the actual wave-field everywhere given the reference wave-field and the perturbation operator; the inverse problem is to construct the perturbation operator (and hence the unknown medium) given the reference wave-field everywhere and the actual wave-field on a measurement surface outside the unknown medium (data). This relation between the three quantities is nonlinear and, to date, it can only be represented using the Born or Neumann series (see e.g. [36]), which, when con-

vergent, constructs the actual wave-field (in the forward problem) and the perturbation operator (in the inverse problem).

The importance and the main use of the forward scattering series until recently came from the application of scattering theory to solving inverse problems. The central tool in this case, the inverse scattering series, is presently the only non-linear, direct inversion method, for the multi-dimensional acoustic or elastic wave equation, which does not require any a priori information about the medium to be investigated. Initially developed by Jost and Kohn [20] and later applied to the seismic problem by Moses in [30], its convergence has been studied, among others, by Prosser [37], who concluded that the convergence of the forward series is necessary for the convergence of the inverse series. From the construction of the inverse series (see e.g. Jost and Kohn [20], Moses [30], Weglein et al. [43]) it is not difficult to see that the convergence of the forward is also necessary for the very existence of the inverse scattering series. As a modeling procedure for the seismic wave-field, the forward scattering series was first studied by Matson [28], for a 1D wave-field propagating in acoustic media, who showed that convergence occurs for a ratio less than $\sqrt{2}$ between the reference and the actual velocity. The study was later extended by Matson [29] and Nita et al. [34] to a 2D wave-field propagating in a vertically varying acoustic medium; they showed that the forward series only converges for either limited velocity contrast or limited incidence angle respectively. Innanen [18] studied the forward scattering series for a 1D wave-field propagating in a visco-acoustic medium and found, consistent with previous results, that the series converges only for a limited contrast between the actual and the reference medium. Ramirez and Otnes [38] have further extended the calculation of the series for the acoustic two parameter (velocity and density) case showing the same limited convergence of the series. Nita [33] showed that, using Padé approximants, it is possible to extend the convergence properties of the one parameter forward scattering series to any velocity contrast for uni-dimensional propagation in both acoustic and visco-acoustic media.

In this paper we use the method presented in [33] to analytically continue the forward scattering series solutions for a simple one dimensional medium embedded in a three dimensional space, and in which only one parameter (velocity) is allowed to vary. We show that using the Padé approximants, and their continued fractions representations, one can extend the solutions to any velocity contrast and to any incidence angle for both acoustic and visco-acoustic media. This extension leads to the construction of post-critical events and headwaves and to their Feynman diagrammatic interpretation in the scattering theory formalism.

Continued fractions have been used before, in a different context, to model seismic wave-field propagation. Jacobs and Muir showed in [19] that Claerbout's 15° and 45° approximations to the square root differential operator, involved in the one-way wave equation (see [12]), are truncations in a continued fractions expansion of that same differential operator (see also [13]). These simplified equations can be used for precise and fast modeling of the scattered field near the source of the wave and are not appropriate for large offsets. Inversely, they can be used as a simplified migration procedure to down-

ward continue the collected data and image the interior of the earth [40]. More recently, Nkemzi and Paul [35] have used Padé approximants to model the scattering amplitude of electromagnetic waves, when interacting with rough surfaces, with excellent numerical results.

The structure of this paper is the following. In Section 2 we briefly present the formalism of the forward scattering series in both operator and functional form and focus on its expression for vertically varying acoustic media. The convergence properties of the series written for one plane wave component are reviewed in Section 3 and the tools for analytically continue these properties (the sequence of Padé approximants and their continued fractions expressions) are also introduced. Section 4 discusses a point-source point-receiver experiment and shows the construction of post-critical waves and refracted wave events (headwaves) from the forward scattering series plane wave solutions. Feynman diagrammatic interpretations of these events in relation to their forward scattering series constructions are presented in Section 5. Conclusions and discussion of future research are included in the final Section 6.

Throughout the paper we use the following conventions for Fourier transforming over the space and time coordinates. For the Fourier transform over the horizontal variable x , we are going to use the different sign convention for the transformation over the source and receiver coordinates. Accordingly, the forward Fourier transform of a real function f over the horizontal source coordinate x_s is going to be

$$f(k_{x_s}) = \int_{-\infty}^{\infty} f(x_s) e^{ik_{x_s}x_s} dx, \quad (1.1)$$

where k_{x_s} is the associated horizontal wavenumber. The forward Fourier transform of f over the horizontal receiver coordinate x_g is going to be

$$f(k_{x_g}) = \int_{-\infty}^{\infty} f(x_g) e^{-ik_{x_g}x_g} dx, \quad (1.2)$$

where k_{x_g} is, same as before, the associated horizontal wavenumber. The associated inverse Fourier transforms are

$$f(x_s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(k_{x_s}) e^{-ik_{x_s}x_s} dx \quad (1.3)$$

and

$$f(x_g) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(k_{x_g}) e^{ik_{x_g}x_g} dx, \quad (1.4)$$

respectively. The forward Fourier transform over the time coordinate t is

$$f(\omega) = \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt, \quad (1.5)$$

where ω is the temporal frequency. Its corresponding inverse Fourier transform will be given by

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega) e^{-i\omega t} d\omega. \quad (1.6)$$

2 Forward scattering series for a vertically varying medium in a 3D space

In operator form, the differential equations describing wave propagation in an actual and a reference medium can be written as

$$\mathbf{L}\mathbf{G} = -\mathbf{I}, \quad (2.1)$$

$$\mathbf{L}_0\mathbf{G}_0 = -\mathbf{I}, \quad (2.2)$$

where \mathbf{L} , \mathbf{L}_0 and \mathbf{G} , \mathbf{G}_0 are the actual and reference differential and Green's operators, respectively, for a single temporal frequency and \mathbf{I} is the identity operator. The above equations (2.1) and (2.2) assume that the source and receiver signatures have been deconvolved. The perturbation, \mathbf{V} , and the scattered field operator, $\boldsymbol{\psi}_s$, are defined as

$$\mathbf{V} = \mathbf{L} - \mathbf{L}_0, \quad (2.3)$$

$$\boldsymbol{\psi}_s = \mathbf{G} - \mathbf{G}_0. \quad (2.4)$$

The fundamental equation of scattering theory, the Lippmann-Schwinger equation, relates $\boldsymbol{\psi}_s$, \mathbf{G}_0 , \mathbf{V} , and \mathbf{G} (see, e.g., [42]):

$$\boldsymbol{\psi}_s = \mathbf{G} - \mathbf{G}_0 = \mathbf{G}_0\mathbf{V}\mathbf{G}. \quad (2.5)$$

Expressions for \mathbf{L} , \mathbf{L}_0 and \mathbf{V} , in the case of a pressure wavefield propagating in inhomogeneous acoustic and elastic media, have been given in [11] and [41]. For a constant density acoustic inhomogeneous medium, case which will be discussed in this paper, these expressions are

$$\mathbf{L} = \nabla + \frac{\omega^2}{c^2(\mathbf{r})}, \quad (2.6)$$

$$\mathbf{L}_0 = \nabla + \frac{\omega^2}{c_0^2}, \quad (2.7)$$

$$\mathbf{V} = \omega^2 \left(\frac{1}{c^2(\mathbf{r})} - \frac{1}{c_0^2} \right), \quad (2.8)$$

where ω is the temporal frequency, $c(\mathbf{r})$ and c_0 are the actual and the reference velocity respectively and \mathbf{r} is the three dimensional position vector.

Eq. (2.5) can be expanded in an infinite series by substituting

$$\mathbf{G} = \mathbf{G}_0 - \mathbf{G}_0\mathbf{V}\mathbf{G}$$

into the right-hand side repeatedly to obtain

$$\boldsymbol{\psi}_s = \mathbf{G}_0\mathbf{V}\mathbf{G}_0 + \mathbf{G}_0\mathbf{V}\mathbf{G}_0\mathbf{V}\mathbf{G}_0, \quad (2.9)$$

$$\boldsymbol{\psi}_s = \mathbf{G}_0\mathbf{V}\mathbf{G}_0 + \mathbf{G}_0\mathbf{V}\mathbf{G}_0\mathbf{V}\mathbf{G}_0 + \mathbf{G}_0\mathbf{V}\mathbf{G}_0\mathbf{V}\mathbf{G}_0\mathbf{V}\mathbf{G}_0,$$

...

and so on. By repeating this process an infinite number of times we imagine that we can drop the last term containing the Green's function of the actual medium, \mathbf{G} , in favor of an infinite series, and write the scattered field as

$$\boldsymbol{\psi}_s \equiv \mathbf{G} - \mathbf{G}_0 = \mathbf{G}_0 \mathbf{V} \mathbf{G}_0 + \mathbf{G}_0 \mathbf{V} \mathbf{G}_0 \mathbf{V} \mathbf{G}_0 + \dots \quad (2.10)$$

When convergent, this series, the forward scattering series, constructs the scattered field operator $\boldsymbol{\psi}_s$ as a sum of terms representing propagations in the reference medium (\mathbf{G}_0) and interactions with the inhomogeneity represented by the perturbation operator \mathbf{V} .

For an acoustic constant density medium, we can define

$$k_0 = \frac{\omega}{c_0}, \quad \alpha(\mathbf{r}) = 1 - \frac{c^2(\mathbf{r})}{c_0^2}$$

and rewrite the perturbation \mathbf{V} as

$$\mathbf{V} = k_0^2 \alpha(\mathbf{r}). \quad (2.11)$$

The forward scattering series then becomes

$$\begin{aligned} \psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) &= \int G_0(\mathbf{r}_g | \mathbf{r}'; \omega) k_0^2 \alpha(\mathbf{r}') G_0(\mathbf{r}' | \mathbf{r}_s; \omega) d\mathbf{r}' \\ &+ \int G_0(\mathbf{r}_g | \mathbf{r}'; \omega) k_0^2 \alpha(\mathbf{r}') \int G_0(\mathbf{r}' | \mathbf{r}''; \omega) k_0^2 \alpha(\mathbf{r}'') G_0(\mathbf{r}'' | \mathbf{r}_s; \omega) d\mathbf{r}'' d\mathbf{r}' \\ &+ \dots, \end{aligned} \quad (2.12)$$

where the integrals are 3D volume integrals taken over the whole space. A physical interpretation of this series was given by [28] and [34]. In this paper we will discuss the single horizontal interface case which, although simplistic, shows the construction of some complex wave events like phase shifted post-critical arrivals and headwaves. For this setting, the perturbation \mathbf{V} becomes

$$\mathbf{V}(z) = k_0^2 \alpha H(z - z_1), \quad (2.13)$$

where $\alpha = 1 - c_1^2/c_0^2$ with c_0 and c_1 representing the speeds of propagation in the two half-spaces, H is the Heaviside function and z_1 the depth of the interface. Eq. (2.12) then becomes

$$\begin{aligned} \psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) &= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy' \int_{z_1}^{\infty} dz' G_0(\mathbf{r}_g | x', y', z'; \omega) k_0^2 \alpha(z') G_0(x', y', z' | \mathbf{r}_s; \omega) \\ &+ \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy' \int_{z_1}^{\infty} dz' G_0(\mathbf{r}_g | x', y', z'; \omega) k_0^2 \alpha(z') \\ &\times \int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dy'' \int_{z_1}^{\infty} dz'' G_0(x', y', z' | x'', y'', z''; \omega) k_0^2 \alpha(z'') \\ &\times G_0(x'', y'', z'' | \mathbf{r}_s; \omega) + \dots \end{aligned} \quad (2.14)$$

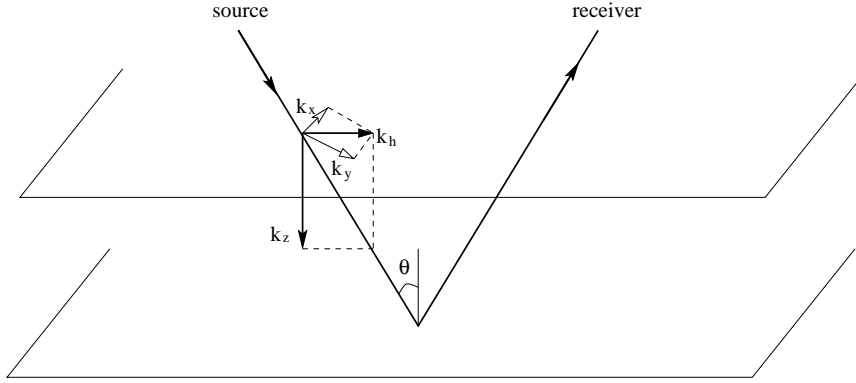


Figure 1: Horizontal and vertical wavenumbers associated with one plane wave component and satisfying the dispersion relation $k_x^2 + k_y^2 + v_0^2 = \omega^2 / c_0^2$. The picture also shows the total horizontal wavenumber, k_h , defined through the relation $k_x^2 + k_y^2 = k_h^2$.

The 3D Green's function representing a spherical wave propagating with velocity c_0 in a homogeneous acoustic medium of constant density is given by (see e.g. [1])

$$G_0(\mathbf{r}_g | \mathbf{r}_s; \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \frac{e^{ik_x(x_g - x_s) + ik_y(y_g - y_s) + i\nu_0|z_g - z_s|}}{i\nu_0}, \quad (2.15)$$

where $\mathbf{r}_s = (x_s, y_s, z_s)$ and $\mathbf{r}_g = (x_g, y_g, z_g)$ are the coordinates for the source and the observation point respectively. The temporal frequency is, as before, denoted by ω , k_x and k_y are the horizontal wavenumbers associated with the x and y coordinates respectively, and ν_0 is the vertical wavenumber satisfying the dispersion relation

$$\nu_0 = \text{sgn}(\omega) \sqrt{\frac{\omega^2}{c_0^2} - k_x^2 - k_y^2}$$

(see Fig. 1). For later use, we also define the cumulative horizontal wavenumber k_h to be

$$k_h^2 = k_x^2 + k_y^2 \quad (2.16)$$

(see Fig. 1). For a non-evanescent plane wave component we can define the angle of incidence θ by the relation

$$\sin \theta = \frac{k_h}{k_0}, \quad (2.17)$$

or, alternatively,

$$\cos \theta = \frac{\nu_0}{k_0}. \quad (2.18)$$

Following [34] we first consider the problem of an incoming plane wave, described by the temporal frequency ω and arbitrary horizontal wavenumbers k_x and k_y , and given by

$$\phi_0(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = e^{i(k_x x_g + k_y y_g + \nu_0 |z_g - z_s|)}. \quad (2.19)$$

With these considerations, we calculate the first term in the forward scattering series in Eq. (2.14) to be

$$\begin{aligned} \psi_s^1(x_g, y_g, z_g | k_x, k_y, z_s; \omega) &= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy' \int_{z_1}^{\infty} dz' k_0^2 \alpha \\ &\times \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_{gx} \int_{-\infty}^{\infty} dk_{gy} \frac{e^{ik_{gx}(x_g-x') + ik_{gy}(y_g-y') + ik_{gz}|z_g-z'|}}{ik_{gz}} e^{ik_x x' + ik_y y' + ik_z |z' - z_s|}. \end{aligned}$$

Since the model we discuss is restricted to vertical variations, the perturbation α also depends only on the depth z . This implies that, in the last formula, we can first integrate over the horizontal coordinates, x' and y' , to obtain two delta functions $\delta(k_{gx} - k_x)$ and $\delta(k_{gy} - k_y)$, and then over the horizontal wavenumbers k_{gx} and k_{gy} , to obtain

$$\psi_s^1(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 2\pi k_0^2 \alpha \frac{e^{ik_x x_g + ik_y y_g}}{ik_z} \int_{z_1}^{\infty} dz' e^{ik_z(2z' - z_g - z_s)}. \quad (2.20)$$

The last integral,

$$\int_{z_1}^{\infty} dz' e^{ik_z(2z' - z_g - z_s)}, \quad (2.21)$$

is not defined in the Riemannian sense because the integrand oscillates, preserving its amplitude, towards infinity. Consistently with [34], we are going to define this integral to be the value of the anti-derivative of the integrand calculated at its finite boundary z_1 , i.e.,

$$\int_{z_1}^{\infty} dz' e^{ik_z(2z' - z_g - z_s)} = -\frac{e^{ik_z(2z_1 - z_g - z_s)}}{2ik_z}. \quad (2.22)$$

As showed in [34], this definition is equivalent with considering that the reference medium attenuates the wave-field which, in consequence, vanishes at infinity. The final expression for ψ_s^1 is

$$\psi_s^1(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 4\pi \frac{k_0^2 \alpha}{v_0^2} e^{ik_x x_g + ik_y y_g + iv_0(2z_1 - z_g - z_s)}. \quad (2.23)$$

Similarly, one can calculate the higher order terms in the forward scattering series ψ_s^i with $i = 1, 2, 3, \dots$, and find

$$\psi_s^2(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 4\pi \frac{1}{8} \left(\frac{k_0^2 \alpha}{v_0^2} \right)^2 e^{ik_x x_g + ik_y y_g + iv_0(2z_1 - z_g - z_s)}, \quad (2.24)$$

$$\psi_s^3(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 4\pi \frac{5}{64} \left(\frac{k_0^2 \alpha}{v_0^2} \right)^3 e^{ik_x x_g + ik_y y_g + iv_0(2z_1 - z_g - z_s)}, \quad (2.25)$$

$$\vdots \quad (2.26)$$

Summing all these terms we find the total scattered field on the measurement surface, produced by the interaction of one plane wave component of a point source, characterized by the horizontal wavenumbers k_x and k_y and the temporal frequency ω , with the interface, to be

$$\begin{aligned} & \psi_s(x_g, y_g, z_g | k_x, k_y, z_s; \omega) \\ &= 4\pi e^{ik_x x_g + ik_y y_g + i\nu_0(2z_1 - z_g - z_s)} \left[\frac{1}{4} \frac{k_0^2 \alpha}{\nu_0^2} + \frac{1}{8} \left(\frac{k_0^2 \alpha}{\nu_0^2} \right)^2 + \frac{5}{64} \left(\frac{k_0^2 \alpha}{\nu_0^2} \right)^3 \dots \right]. \end{aligned} \quad (2.27)$$

The modeled wavefield (data) should consist of primary (single) reflections and internal and free surface multiple reflections (reverberations) when the geometry of the model permits it (two interfaces or more and a free surface respectively). However, in this case, since the solutions are represented as a series, the convergence of the forward scattering series is also a necessary condition for the method to work. In the next section we briefly review the convergence properties of this infinite series in terms of the characteristics of the plane wave component (horizontal and vertical wavenumbers and/or angle of incidence).

3 Convergence properties of the forward scattering series

The expression (2.27) is easily compared with Eq. (3.15) in [34]. When convergent, the expression in parenthesis constructs the angle dependent reflection coefficient associated with the contrast in velocity at the interface. The convergence properties for this series have been discussed in Nita et al [34], which concluded that it is dependent on the angle of incidence (here defined in Eqs. (2.17) and (2.18)) of the plane wave onto the interface. Their results can be summarized as follows. For plane waves arriving at pre-critical and critical angles, $\theta \leq \theta_c = \sin^{-1}(c_0/c_1)$, the series converges and it constructs the angle dependent reflection coefficient

$$R = \frac{\nu_1 - \nu_0}{\nu_1 + \nu_0}, \quad (3.1)$$

where ν_1 and ν_0 are the vertical wavenumbers defined by

$$\nu_1 = \sqrt{\omega^2/c_1^2 - k_x^2 - k_y^2}, \quad (3.2)$$

$$\nu_0 = \sqrt{\omega^2/c_0^2 - k_x^2 - k_y^2}. \quad (3.3)$$

The expression (2.27) of the scattered field due to an incoming plane wave described by k_x , k_y and ω becomes in this case

$$\psi_s(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 2\pi R e^{ik_x x_g + ik_y y_g + i\nu_0(2z_1 - z_g - z_s)}. \quad (3.4)$$

For plane waves arriving at post-critical angles, $\theta > \theta_c = \sin^{-1}(c_0/c_1)$, the series diverges and hence the forward scattering series fails to construct the scattered field. The

reasoning behind this limitation of the method was explained in [33]. Roughly speaking, the divergence occurs because of the iterative construction of the forward scattering series from the Lippmann-Schwinger relationship (2.5) and the dropping of the last term containing the actual medium's Green's function \mathbf{G} in Eq. (2.9) in favor of the infinite series in Eq. (2.10). Nita showed in [33] that this partial solution can, however, be extended by using a combination of Padé approximants and continued fractions approach. In the following, we apply this method to the vertically varying three dimensional model described above to analytically continue the forward scattering series solutions beyond their domain of convergence.

By definition, a Padé approximant to the power series $\sum a_n x^n$ is a rational expression

$$P_M^N(x) = \frac{\sum_{n=0}^N A_n x^n}{\sum_{n=0}^M B_n x^n} \tag{3.5}$$

whose Taylor series representation coincides with the series up to $(N+M+1)-th$ order. For a discussion of their properties and applications see e.g. [4]. For a 1D acoustic or visco-acoustic medium and a normally incident plane wave onto one interface, Nita shows in [33] that the sequence of Padé approximants $P_0^0, P_1^0, P_1^1, P_2^1, P_2^2, P_3^2, \dots$ converges to the exact value of the reflection coefficient for any velocity contrast.

For an arbitrary plane wave, incident onto the interface at an angle θ , the discussion is similar to the vertical incidence case, with the exception of the extra factor k_0^2/v_0^2 (which equals to 1 for the normal incidence case). Following [33] we can hence calculate

$$P_0^0 = 0, \tag{3.6}$$

$$\vdots$$

$$P_2^1 = \frac{\frac{1}{2} - \frac{1}{4}x}{1 - \frac{3}{4}x + \frac{1}{16}x^2}, \tag{3.7}$$

$$P_2^2 = \frac{\frac{1}{8}x - \frac{1}{16}x^2}{1 - x + \frac{3}{16}x^2}, \tag{3.8}$$

$$\vdots$$

$$P_4^3 = \frac{\frac{1}{8}x - \frac{7}{48}x^2 + \frac{7}{192}x^3}{1 - \frac{5}{3}x + \frac{13}{16}x^2 - \frac{5}{48}x^3 - \frac{1}{768}x^4}, \tag{3.9}$$

$$\vdots$$

$$P_5^5 = \frac{\frac{1}{8}x - \frac{1}{4}x^2 + \frac{21}{128}x^3 - \frac{5}{128}x^4 + \frac{5}{2048}x^5}{1 - \frac{5}{2}x + \frac{9}{4}x^2 - \frac{7}{8}x^3 + \frac{35}{256}x^4 - \frac{3}{512}x^5}, \tag{3.10}$$

and so on, where $x = k_0^2 \alpha / v_0^2$ is the normalized secant of the incidence angle. Each Padé approximant in the sequence above provides a more accurate value for the amplitude

of the scattered wavefield than the forward scattering series. At each step, for example, we can then compute different orders of approximations of the scattered field using the formula

$$(\psi_s)_{M+N}(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 4\pi P_M^N e^{ik_x x_g + ik_y y_g + iv_0(2z_1 - z_g - z_s)}, \quad (3.11)$$

where P_M^N represents the Padé approximation to the reflection coefficient with $M = N$ or $M = N + 1$ (compare with Eq. (3.4)). By definition, the Taylor series for P_M^N coincides with the forward scattering series up to the $(N + M + 1) - th$ but it has different terms for higher orders. Those different terms are able to counteract the divergence introduced by dropping the actual medium's Green's function \mathbf{G} in Eq. (2.9) in favor of the infinite series in Eq. (2.10). The result is a sequence of approximants which converges to the actual value of the scattering amplitude for all contrasts between the actual and the reference medium and all incidence angles.

The downside of using Padé approximants is that, at each step, one has to calculate $(N + M + 1)$ new coefficients without being able to recycle the ones calculated for lower orders. However, the special sequence of approximants in Eqs. (3.6)-(3.10) has a continued fractions representation of the form

$$F_N(x) = \frac{c_0}{1 + \frac{c_1 x}{1 + \frac{c_2 x}{1 + \dots \frac{c_{N-1} x}{1 + c_N x}}}}, \quad (3.12)$$

where x , as before, is the normalized secant of the incidence angle $x = k_0^2 \alpha / v_0^2$. The sequence of Padé approximants $P_0^0, P_1^0, P_1^1, P_2^1, P_2^2, P_3^2, \dots$, considered above is called normal if every member exists and no two members are identically equal. It can be shown that if this Padé sequence is normal, then the $(N + 1)th$ term has the continued fraction representation (3.12) with the coefficients c_n being the same for every term of the sequence. In other words, $P_{M+1}^M(x)$, for $M > 0$, is obtained from $P_M^M(x)$ by simply replacing $c_N x$ by $c_N x / (1 + c_{N+1} x)$ where $N = 2M$, and $P_{M+1}^{M+1}(x)$, for $M \geq 0$, is obtained from $P_{M+1}^M(x)$ by replacing $c_N x$ by $c_N x / (1 + c_{N+1} x)$ where $N = 2M + 1$. For the seismic model considered here, following Nita [33], we can write

$$f_n(x) = \frac{1/4}{1 - x f_{n-1}(x)}, \quad (3.13)$$

where either $f_n = P_N^N$ if n is even and $n = 2N$ or $f_n = P_{N+1}^N$ if n is odd and $n = 2N + 1$. This relation provides a fast iterative scheme to calculate the Padé approximants to any order. In addition, we reiterate the fact that, in contrast to the Padé approximants representation as a ratio of two polynomials, where, for each higher rank, every coefficient in the rational fraction must be recomputed, in this representation, only one new coefficient need be computed as we go from one term in the sequence to the next.

Using the arguments presented in [33], one can show the convergence of the sequence of continued fractions or, equivalently, the convergence of the sequence of Padé approximants for any value of $k_0^2\alpha/v_0^2$ in the complex plane, except the cut from 1 to ∞ along the real axis. On this branch-cut, we have $k_0^2\alpha/v_0^2 \geq 0$ which is equivalent to having

$$\left(\frac{v_1}{v_0}\right)^2 \leq 0, \tag{3.14}$$

where v_1 and v_0 are the vertical wavenumbers of the actual and the reference media respectively,

$$v_1 = \sqrt{\omega^2/c_1^2 - k_h^2}, \quad v_0 = \sqrt{\omega^2/c_0^2 - k_h^2}.$$

For post-critical incident plane waves, v_1 becomes imaginary and the condition in equation (3.14) is satisfied which implies the sequence of Padé approximants above will not converge. To circumvent this apparent problem, we can consider an attenuating actual medium by introducing an additional imaginary part in the velocity c_1 through the relation (see e.g. [1])

$$\frac{1}{c_1^{new}} = \frac{1}{c_1} + i\epsilon, \tag{3.15}$$

with ϵ being a small parameter such that $\epsilon > 0$ for $\omega > 0$. Since all real media have some attenuation property, the introduction of this new effective velocity only makes the method more realistic. It is easy to see that the quantity $k_0^2\alpha/v_0^2$ is now complex (and so no longer along the branch-cut), and hence the condition (3.14) is never satisfied. This implies that the sequence of Padé approximants for this model converges for all velocity contrasts and all incidence angles.

In addition, the limit of Padé approximants in Eqs. (3.6)-(3.10) turns out to be

$$\frac{v_0^2}{k_0^2\alpha} \left(1 - \frac{1}{2} \frac{k_0^2\alpha}{v_0^2} - \sqrt{1 - \frac{k_0^2\alpha}{v_0^2}} \right) = \frac{1}{2} \frac{v_1 - v_0}{v_1 + v_0}, \tag{3.16}$$

where v_1 is the vertical wavenumber of a particular plane wave component propagating through the second medium, c_1 , and satisfying

$$v_1^2 = \frac{\omega^2}{c_1^2} - k_h^2.$$

This expression is recognized to be the angle dependent reflection coefficient (see e.g. [1]) and so the full expression of the scattered field produced by an incident plane wave component at arbitrary incidence angle becomes

$$\psi_s(x_g, y_g, z_g | k_x, k_y, z_s; \omega) = 2\pi R e^{ik_x x_g + ik_y y_g + iv_0(2z_1 - z_g - z_s)}. \tag{3.17}$$

The convergence of the sequence of Padé approximants allows the construction of the angle dependent reflection coefficient at any incident angle, and implicitly, the scattered field for a point-source and point-receiver experiment. This construction will be discussed in the following section.

4 A point source experiment

To obtain the scattered field from a point source - point receiver experiment one has to add together the scattered field created by all plane wave components with the appropriate weighting

$$\psi_s(\mathbf{r}_g|\mathbf{r}_s;\omega) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y e^{-i(k_x x_s + k_y y_s)} \frac{\psi_s(x_g, y_g, z_g | k_x, k_y, z_s; \omega)}{2iv_0}, \quad (4.1)$$

where $\mathbf{r}_g = (x_g, y_g, z_g)$ and $\mathbf{r}_s = (x_s, y_s, z_s)$. Notice that this integration was not possible with the solution obtained from the forward scattering series alone, since the expression was divergent for large angles plane wave components. The solution obtained using Padé approximants converges for all wavenumbers and allows the integration and hence the construction of a point source response. Substituting the expression (3.17) into Eq. (4.1)

$$\psi_s(\mathbf{r}_g|\mathbf{r}_s;\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \frac{R e^{i(k_x(x_g - x_s) + k_y(y_g - y_s) + v_0(2z_1 - z_g - z_s))}}{iv_0}, \quad (4.2)$$

where R is the angle dependent reflection coefficient.

To integrate the above expression we first change the integration variables (k_x, k_y) to cylindrical coordinates (k_h, ϕ) to obtain the Sommerfeld integral form. To that end we let

$$k_x = k_h \cos \phi', \quad k_y = k_h \sin \phi' \quad (4.3)$$

and notice that the Jacobian for this transformation is k_h and so $dk_x dk_y = k_h dk_h d\phi'$. With the new ranges $0 \leq k_h < \infty$ and $0 \leq \phi' < 2\pi$ the expression (4.2) becomes

$$\psi_s(\mathbf{r}_g|\mathbf{r}_s;\omega) = \frac{1}{2\pi} \int_0^{\infty} dk_h \frac{R k_h J_0(k_h h) e^{iv_0(2z_1 - z_g - z_s)}}{iv_0}, \quad (4.4)$$

where the Cartesian coordinates (x, y) were changed to polar coordinates, offset-azimuthal angle (h, ϕ) , using $x = h \cos \phi$ and $y = h \sin \phi$ and we have introduced the Bessel function of the first type

$$J_0(k_h h) = \frac{1}{2\pi} \int_0^{2\pi} d\Phi e^{ik_h h \cos \Phi}. \quad (4.5)$$

The expression can further be simplified by changing integration variable in (4.4) from the horizontal wavenumber k_h to the horizontal slowness or ray parameter p related through $k_h = \omega p$. The mapping between the (k_h, ω) to (p, ω) domain has been studied extensively by Bracewell (see [5, 6]). It mainly consists in reading the data along the lines going through the origin of the (k_h, ω) coordinate system instead of the original (k_h, ω) grid (see Fig. 2).

With this change, the scattered field can be written as

$$\psi_s(\mathbf{r}_g|\mathbf{r}_s;\omega) = i\omega \int_0^{\infty} dp \frac{R p J_0(\omega p h) e^{i\omega \zeta (2z_1 - z_g - z_s)}}{i\zeta}, \quad (4.6)$$

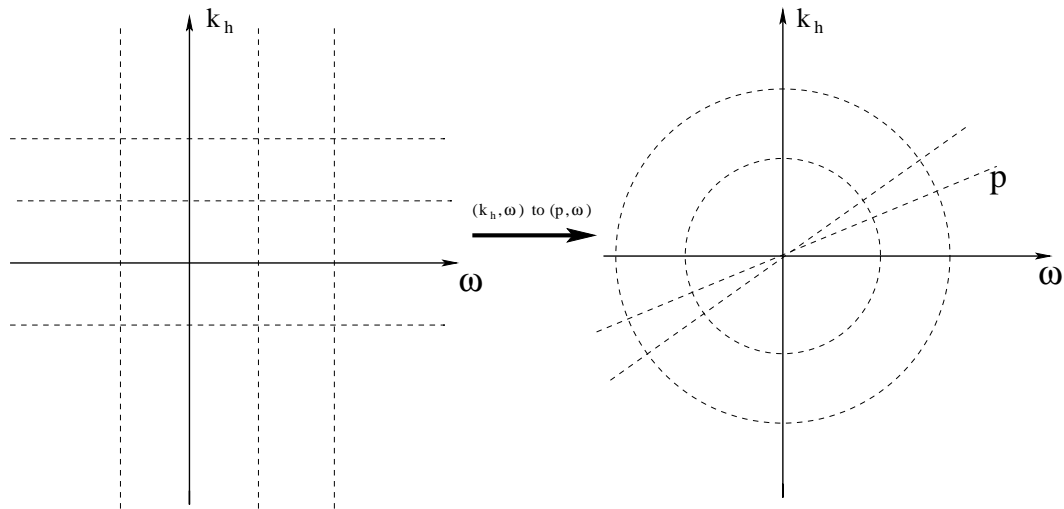


Figure 2: The mapping (k_h, ω) to (p, ω) .

where $\zeta = \sqrt{c_0^{-2} - p^2}$. We can rewrite the integral above using Hankel functions of the first type, $H_0^{(1)}$, as

$$\psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) = \frac{1}{2} i \omega \int_{-\infty}^{\infty} dp \frac{Rp H_0^{(1)}(\omega p h) e^{i \omega \zeta (2z_1 - z_g - z_s)}}{i \zeta} \tag{4.7}$$

and use the asymptotic approximation of the first order

$$H_0^{(1)} = \sqrt{\frac{2}{\pi \omega p h}} e^{i \omega p h} e^{-i \pi / 4} \tag{4.8}$$

to simplify the expression to

$$\psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) = \frac{e^{-i \pi / 4}}{2} i \omega \int_{-\infty}^{\infty} dp \sqrt{\frac{2}{\pi \omega p h}} e^{i \omega p h} \frac{Rp e^{i \omega \zeta (2z_1 - z_g - z_s)}}{i \zeta}. \tag{4.9}$$

This integral can be solved numerically with very accurate results. However, for the sake of interpretation, we are going to briefly look at how to solve it analytically using the saddle point approximation method after distorting the path of integration to avoid the three branch-cut singularities in the complex p plane. Recall that the formula for this type of approximation is

$$\int dk_h e^{i \omega f(p)} \approx \sqrt{\frac{2 \pi i}{\omega f''(p_s)}} e^{i \omega f(p_s)}, \tag{4.10}$$

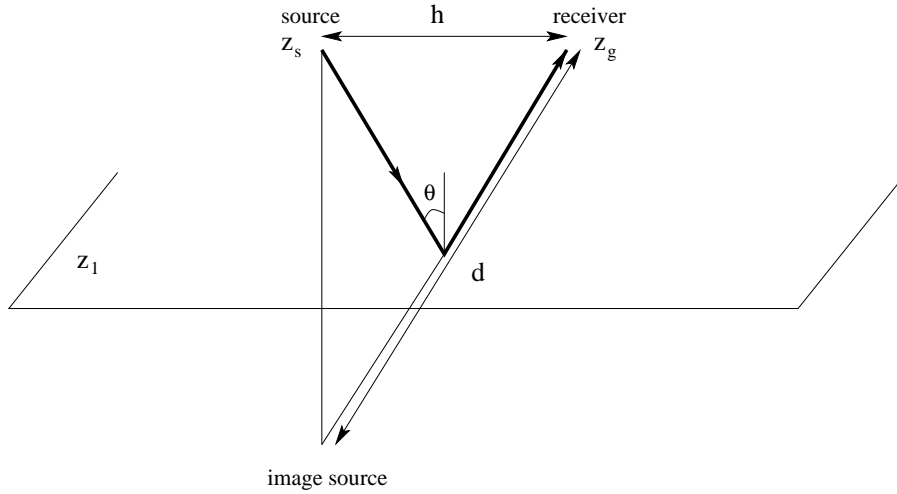


Figure 3: The main contribution in the saddle point approximation for the scattered field for the $c_0 > c_1$ and pre-critical $c_0 < c_1$ cases. In this picture h represents the horizontal offset and d represents the total distance traveled by the wave from source to interface to receiver.

where p_s is the root of $f'(p) = 0$. Using this formula (the details can be found for example in [1]), we find, for $c_0 > c_1$,

$$\psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) \approx \frac{R(p_s)}{d} e^{i\omega t_R} \quad (4.11)$$

with $t_R = d/c_0$ being the total traveltime of the reflection (see Fig. 3). When $c_0 < c_1$, the situation is more complicated, and the use of Eq. (4.10) has to take into consideration several possibilities for the position of the saddle point p_s on the real p axis. The discussion is equivalent to considering the pre-critical and post-critical offsets between the source and receiver in the experiment. For pre-critical we have

$$\psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) \approx \frac{R(p_s)}{d} e^{i\omega t_R}, \quad (4.12)$$

which is essentially the same result as for the $c_0 > c_1$ case (see also Fig. 3). For the post-critical case the integration path has to be distorted in a more complex way (see e.g. [1]) and an extra contribution appears due to an integration around one of the branch cut singularities. This extra contribution describes the appearance of a, what is called in seismology, conical wave or lateral wave or headwave. The expression of the scattered field in this case is

$$\psi_s(\mathbf{r}_g | \mathbf{r}_s; \omega) \approx \frac{R(p_s)}{d} e^{i\omega t_R} + \frac{2i}{\omega} \frac{c_0^2}{c_1 \alpha} \frac{1}{\sqrt{hL^{3/2}}} e^{i\omega t_H}, \quad (4.13)$$

where L is the horizontal part in the ray-like path of the headwave and, for large offsets, can be approximated by h . The analytical derivation of Eqs. (4.11)-(4.13) provide excellent

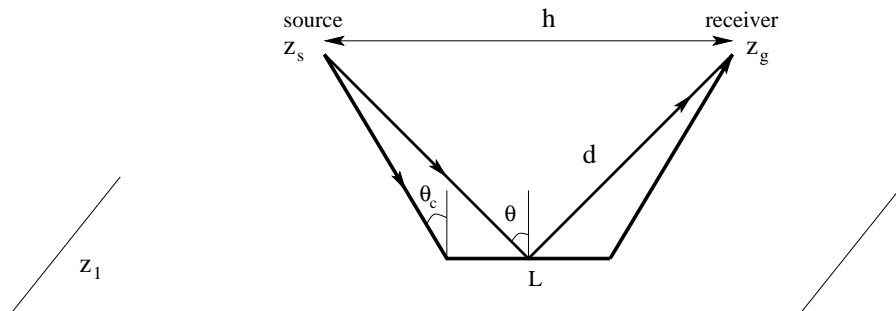


Figure 4: The main contribution in the saddle point approximation for the scattered field for the post-critical $c_0 < c_1$ case. In this picture h represents the horizontal offset, d represents the total distance traveled by the reflected wave from source to interface to receiver and L is the horizontal part (along the interface) in the path of the headwave.

insights into the physical interpretation of the results. For the $c_0 > c_1$ and pre-critical $c_0 < c_1$ cases, the main contribution in the reflection event arrives from the plane wave component incident at the angle $\theta = \tan^{-1}(h/2z)$. For post-critical $c_0 < c_1$ case, we have two distinct events in the data: a reflection for which the main contribution comes, as before, from the plane wave component incident at the post-critical angle $\theta = \tan^{-1}(h/2z)$ and a headwave, which combines contributions from all post-critically incident plane waves with the most important one coming from the critical incident one. These insights can be applied to the point-scatterer model of the medium to obtain scattering theory descriptions of pre- and post-critically reflected waves and refracted waves (headwaves).

Eq. (4.1) can also be solved using the approximation to the scattered wavefield given by the expression in (3.11). Although an approximation, the numerical results described in [33] indicate two types of advantages when using this latter approach. First the low orders of Padé approximants can approximate extremely well the actual values of the reflection coefficient. In conclusion, one can work with the simpler function given by a Padé approximant (rational function) instead of the actual reflection coefficient (irrational function). Second, the discrete zeros of Padé approximants reconstruct the branch-cut singularity of the reflection coefficient responsible for the expression of the headwave in Eq. (4.13). The lower the order of a Padé approximant, the lower the number of singularities to integrate, and hence the faster the procedure and the modeling algorithm.

For the example described above, the complete modeling method could hence be described in three steps:

1. Model the response of the medium using the forward scattering series for an arbitrary incoming plane wave component.
2. Use the method of Padé approximants to obtain a complete representation and a better approximation of the scattered field. Speed up the numerical calculation of the approximants by using the continued fractions expressions.
3. Perform a weighted plane wave summation to construct the impulse response from a point source.

The example described above is for the simple case of an acoustic medium with one parameter (velocity) varying and one single interface. In the last section, Discussion and Conclusions, we will describe a generalization of the procedure to the multi-interface and multi-dimensional cases which will be the object of future research.

5 Scattering theory diagrammatic interpretation

The discussion above can be implemented at the point scatterer level to provide scattering theory diagrammatic representations for pre- and post-critical reflections and head-waves. Recall (see e.g. [28,29,34]) that forward scattering series in Eq. (2.10)

$$\psi_s \equiv \mathbf{G} - \mathbf{G}_0 = \mathbf{G}_0 \mathbf{V} \mathbf{G}_0 + \mathbf{G}_0 \mathbf{V} \mathbf{G}_0 \mathbf{V} \mathbf{G}_0 + \dots \quad (5.1)$$

has a very simple and powerful physical interpretation. Usually, one considers the perturbation \mathbf{V} to be composed of infinitely many point scatterers embedded in the reference medium. The first term in the series can be thought of representing a summation over all 1-interaction events, i.e. events with only one interaction with a point scatterer in their history. The second term represents a summation over all 2-interaction events and so on. As it can be seen from the series, all propagations between source, receiver and scatterers occur only in the reference medium, i.e., with the Greens function \mathbf{G}_0 , even though the speed of the wave in the actual medium is different from the speed of the wave in the reference medium. A diagrammatic representation of these interactions is shown in Fig. 5. In [34], Nita et al. show how to calculate the terms in the forward scattering series for an acoustic medium with a single interface using far field approximations. The analysis in the previous sections, extends the physical interpretation and diagrams included in [34] to the following cases.

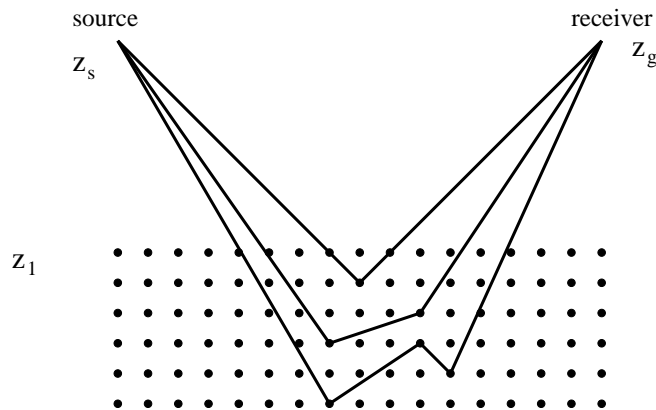


Figure 5: Diagrammatic representation of the point-scatterer interactions described by the forward scattering series. 1-, 2- and 3-interactions are shown with propagations from the source to the scatterers, between scatterers and from the scatterers to the receiver in the reference medium only.

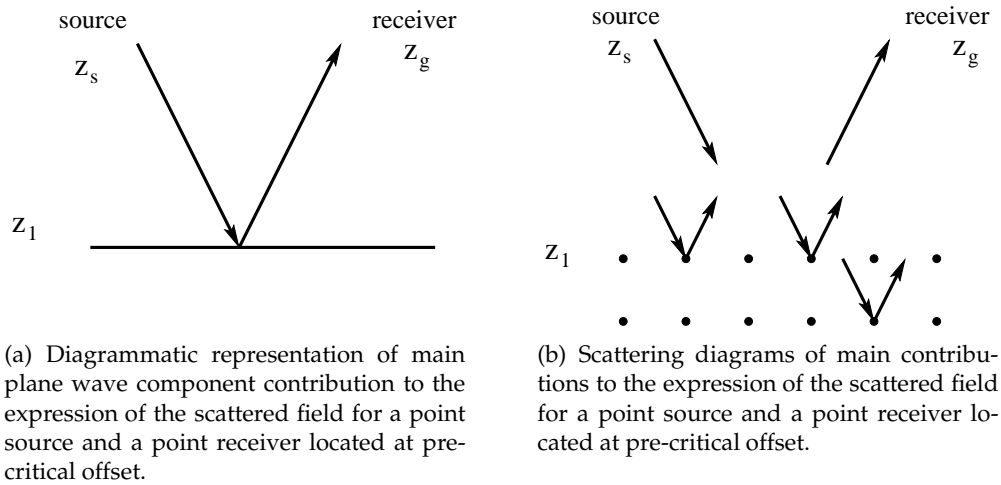


Figure 6: Pre-critical diagrams.

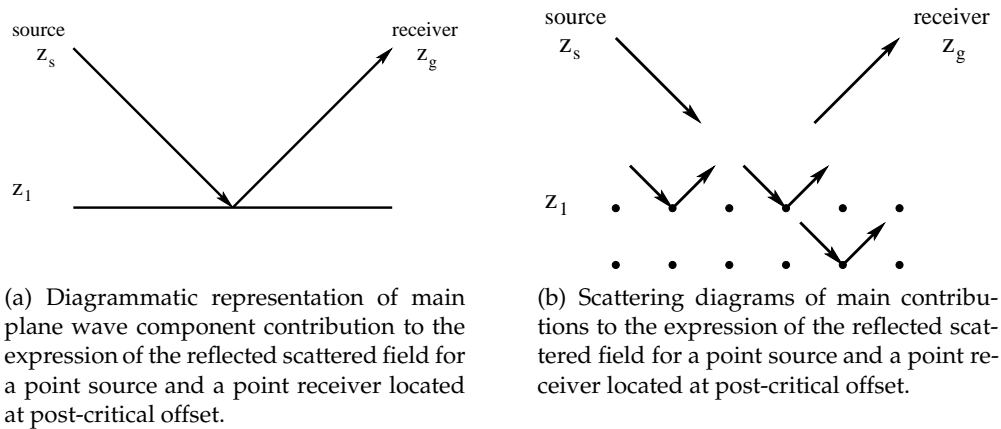


Figure 7: Post-critical diagrams.

For pre-critical offsets, the contribution of a plane wave component comes from ray-like diagrams which share the same (pre-critical) angle of incidence and reflection as the incoming plane wave (see Fig. 6). Summing all the different orders of interaction in the forward scattering series one can find the medium's response to that incoming plane wave component. For a point source and a point receiver located at pre-critical offset, the main contribution is given by the plane wave whose ray-like path satisfies the Snell's Law, i.e., for which the incidence angle is equal to the reflection angle. For this case, after performing a saddle point approximation, we arrive at the expression for the pre-critically scattered field given in Eq. (4.12).

For post-critical reflections, the situation is similar to the pre-critical case, only now

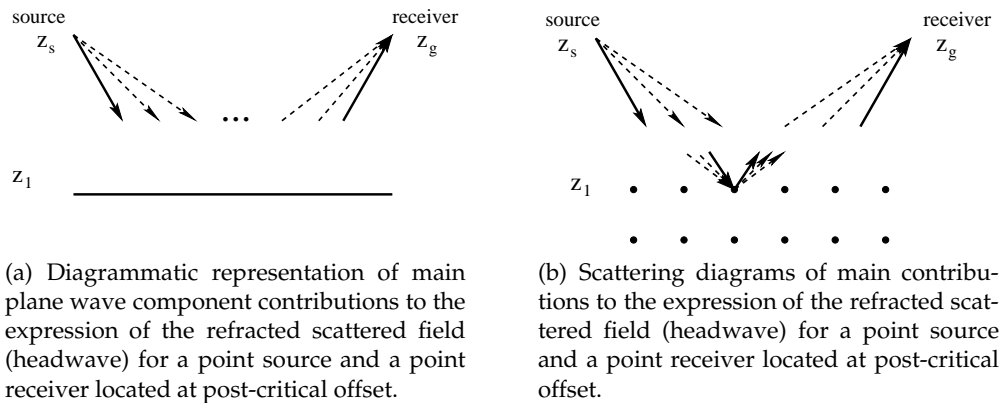


Figure 8: Headwaves diagrams.

the contributions to the scattered field are made by the post-critical scattering diagrams with the same (post-critical) angle of incidence and reflection as the incoming plane wave component (see Fig. 7). To find the medium's response to one post-critical plane wave component, one has to sum all the terms in the forward scattering series using Padé approximants. For a point source and a point receiver located at post-critical distance, the main contribution will be given by the plane wave component whose ray-like path satisfies Snell's Law. For this case, after performing a saddle point approximation, we arrive at the expression for the post-critically reflected wavefield given in the first part of Eq. (4.13).

For post-critical refractions (headwaves) the contributions to the scattered field are made by the plane waves arriving at the critical (main contribution) and post-critical angles. As before, to find the medium's response to one post-critical plane wave component, one has to sum all the terms in the forward scattering series using Padé approximants. For a point source and a point receiver located at post-critical distance, the main contributions will be given by the plane wave components whose ray-like paths satisfy Snell's Law with the angle of incidence/reflection equal to the critical angle characteristic to that interface. For this case, after performing a saddle point approximation, we arrive at the expression for the post-critically refracted wavefield given in the second part of Eq. (4.13).

6 Discussion and conclusions

In this paper we presented the application of the theory of Padé approximants and continued fractions to extend the scattering theory solutions for the acoustic wave equation for a vertically varying 3D medium. We have assumed that only one parameter, velocity, varies and that the medium is composed of two infinite half spaces. Although simplistic, the model shows the power of the Padé approximants to describe both well behaved

amplitudes and singularities and extend the construction of the full scattered field to a point-source experiment, including complicated wave events like headwaves. A key point in the method presented above, was the relation between the forward scattering series and a special sequence of Padé approximants with its corresponding continued fractions expression. This relation was possible because the forward scattering series for the model used in the previous example proved to be a Taylor series for the scattered field as a function of the velocity perturbation. The extension of the method to more complex higher dimensional media also depends on this property. In the following we describe a possible multi-dimensional approach to calculating the forward scattering series and interpreting it as a Taylor series.

For an acoustic multi-dimensional medium, following [23] we can define the set \mathbf{M} of model parameters to be the space of complex valued functions defined on a bounded domain Ω and bounded almost everywhere, i.e. $\mathbf{M} \subset L^\infty(\Omega)$. The norm on this space is the essential supremum given by

$$\|m\|_\infty = \inf \{B : |m(\mathbf{r})| < B \text{ a.e. on } \Omega\}. \quad (6.1)$$

Suppose we fix one of these model parameters (the one describing the reference medium) and let \mathbf{G}_0 , as before, be the Green's function describing wave propagation in this medium

$$(\nabla^2 + m_0)\mathbf{G}_0 = \delta(\mathbf{r} - \mathbf{r}_0), \quad (6.2)$$

where \mathbf{r} and \mathbf{r}_0 are points in Ω . Examples of model parameters describing the acoustic case have been given in Eqs. (2.6), (2.7) and (2.8). Under the condition that

$$\int_\Omega \int_\Omega |\mathbf{G}_0(\mathbf{r}, \mathbf{r}_0, k, m_0)|^2 < C \quad (6.3)$$

for a certain constant C , we can define a directional derivative of the scattered field as a function of the model parameter m , and calculated at m_0 , using the formula (see [23])

$$\psi'(m_0)\Delta m = -k^2 \int_\Omega \mathbf{G}_0(\mathbf{r}_g, \mathbf{r}', m_0) \mathbf{V}(\mathbf{r}') \mathbf{G}_0(\mathbf{r}', \mathbf{r}_s, m_0) dx', \quad (6.4)$$

where we denoted by \mathbf{V} the difference between the actual and the reference model parameter $m - m_0$. With this definition we can compute the second derivative of the scattered field as a function of the model parameter m calculated at m_0 to be

$$\begin{aligned} & \frac{1}{2} \psi''(m_0) \Delta m \\ &= -k^2 \int_\Omega \mathbf{G}_0(\mathbf{r}_g, \mathbf{r}', m_0) \mathbf{V}(\mathbf{r}') \left[\int_\Omega \mathbf{G}_0(\mathbf{r}', \mathbf{r}'', m_0) \mathbf{V}(\mathbf{r}'') \mathbf{G}_0(\mathbf{r}'', \mathbf{r}_s, m_0) d\mathbf{r}'' \right] d\mathbf{r}', \quad (6.5) \end{aligned}$$

and so on up to any order of differentiation. The result from this calculation builds up terms in the forward scattering series given in Eq. (2.10): Eq. (6.4) represents the first term

in the forward scattering series, Eq. (6.5) is the second term and so on. Moreover, with the new definition of directional derivative, it is now possible to write the forward scattering series as a Taylor series for the scattered field as a function of the actual model parameter m calculated at the reference model parameter m_0

$$\psi(m) = \psi(m_0) + \frac{1}{2}\psi'(m_0)(m - m_0) + \dots \quad (6.6)$$

Similar to the 1D case, this is a Taylor series with limited convergence properties dictated by the degree of separation between the reference and the actual model. Based on the results presented in the previous section, we expect that this Taylor series can also be analytically continued using a method based on the special sequence of Padé approximants to extend its convergence to any contrast between the reference and the actual medium. Depending on the choice of the model parameters m , the series in Eq. (6.6) covers 1D single and multiple interfaces, and multi-dimensional acoustic media. These topics along with numerical tests and the possibility of using the Padé approximants and the continued fractions in solving the inverse problem, and in connection with the inverse scattering series, will be studied in future research.

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