Exact wave field simulation for finite-volume scattering problems

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Abstract: An exact boundary condition is presented for scattering problems involving spatially limited perturbations of arbitrary magnitude to a background model in generally inhomogeneous acoustic media. The boundary condition decouples the wave propagation on a perturbed domain while maintaining all interactions with the background model, thus eliminating the need to regenerate the wave field response on the full model. The method, which is explicit, relies on a Kirchhoff-type integral extrapolation to update the boundary condition at every time step of the simulation. The Green's functions required for extrapolation through the background model are computed efficiently using wave field interferometry.

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1. Introduction

Many problems involving wave scattering such as wave form inversion, experimental and industrial design, and nondestructive testing, require evaluation of the wave field response for a suite of closely related models. While these models define material property distributions over some volume V, changes between models may be restricted to a smaller subvolume $D_{\rm sct}$. Nevertheless, repeated full wave form simulations for each entire model are often a necessity as realistic strong multiple scattering rules out a Born approximation. This situation arises, for example, in complex, multibody scattering problems where only one of the bodies changes shape, material properties, or orientation (Schuster, 1985), or when the changes occur in the vicinity of a free surface or otherwise strong scatterers such as fault planes (Robertsson and Chapman, 2000). We suggest that this paradigm may be broken by combining a Kirchhoff-type integral extrapolation with recent advances in wave field interferometry, resulting in an exact boundary condition for model perturbations of arbitrary magnitude, shape, and size. This allows wave field simulations to be restricted to a subdomain enclosing the changes while retaining all interactions with the full volume.

Nonreflecting boundary conditions based on the Kirchhoff integral were first proposed by Ting and Miksis (1986). By extrapolating the wave field from an artificial surface surrounding a scatterer to the boundary of the computational domain, exact boundary conditions were found such that the computational domain could be truncated without generating spurious boundary reflections. The boundary condition was implemented and tested by Givoli and Co-

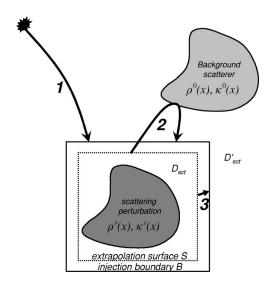


Fig. 1. Definition of the extrapolation surface S and injection boundary B. Note that three events will contribute to the boundary condition as denoted by arrows: (1) The incident wave field propagating in the background medium, (2) the extrapolated waves that are incoming at the boundary and which radiate back into the subgrid, providing long-range interactions, and (3) the extrapolated waves that are outgoing at the boundary (these will complement the corresponding waves propagating on the subgrid).

hen (1995). Exploring the limiting case where the extrapolation surface coincides with the boundary condition, Teng (2003) obtained a boundary integral equation that could be solved in conjunction with the finite-difference scheme on the subgrid. However, in each case, only exterior (outgoing) wave problems were considered, with nonreflecting boundary conditions outside the scatterer.

On the other hand, if one considers locally perturbed scattering problems, the boundary condition between perturbed and unperturbed domains should treat both incoming and outgoing waves correctly. Schuster (1985) proposes a hybrid boundary integral equation plus Born series modeling scheme that accounts for the long-range interactions between a scattering perturbation and the background by solving a surface boundary integral equation, and which represents the interaction between perturbations using a Born series. However, only homogeneous backgrounds and interiors were considered. Finally, Robertsson and Chapman (2000) describe a method to "inject" a wave field recorded during an initial simulation on the full background model, which then drives the computation on the perturbed interior domain. Their boundary condition correctly accounts for the interaction of the wave field on the subvolume, and between the subvolume and the unperturbed background model, both of which can be arbitrarily heterogeneous. The only part of the wave field missing is that caused by interactions of the altered wave field with the unaltered model outside the subvolume which propagate back into the subvolume and interact with the perturbations again—so-called high-order, long-range interactions (Fig. 1, label 2)

The exact boundary condition presented here combines elements from the "injection" and Kirchhoff extrapolation approaches: It uses an incident wave field as a boundary condition to drive the simulation on the subvolume, but accurately models all high-order, long-range interactions between the perturbed region and the background medium by updating the boundary condition through the evaluation of a Kirchhoff-type integral involving full wave form Green's functions.

One of the main contributions of this letter, and a key enabler for the new method, is the realization that the Green's functions required for extrapolation through the background model can be computed efficiently and flexibly using recent advances in wave field interferometry: By illuminating the model from a surrounding surface with a sequence of conventional forward modeling runs, exact Green's functions between any pair of points can be computed using only cross correlations and summations (Wapenaar, 2004; van Manen *et al.*, 2005).

2. Scattering by an arbitrary inhomogeneous object

It is well known how the wave field scattered by an object with mass density $\rho^{s}(\mathbf{x})$ and compressibility $\kappa^{s}(\mathbf{x})$, different from properties $\rho^{0}(x)$, $\kappa^{0}(x)$ of the inhomogeneous medium within which it is embedded, originates from the contrast in the material properties. Defining the scattered wave field $\{p^{\text{sct}}, v_k^{\text{sct}}\}$ as the difference between the total wave field $\{p, v_k\}$ propagating in the perturbed model, and the incident wave field $\{p^{\text{inc}}, v_k^{\text{inc}}\}$ propagating in the background model, it is straightforward to show that the scattered wave field quantities satisfy (Fokkema and van den Berg, 1993):

$$\partial_k p^{\text{sct}} + \rho^0 \partial_t v_k^{\text{sct}} = (\rho^0 - \rho^s) \partial_t v_k, \quad \mathbf{x} \in D_{\text{sct}}, \tag{1}$$

$$\partial_t v_t^{\text{sct}} + \kappa^0 \partial_t p^{\text{sct}} = (\kappa^0 - \kappa^s) \partial_t p, \quad \mathbf{x} \in D_{\text{sct}},$$
 (2)

where ∂_k and ∂_t denote partial derivatives with respect to the kth spatial dimension ($k \in 1,2,3$) and time, respectively, and the Einstein summation convention for repeated indices is used. Equations (1) and (2), show how the scattered wave field originates from body force sources, ($\rho^0 - \rho^s$) $\partial_t v_k$, and volume injection sources, ($\kappa^0 - \kappa^s$) $\partial_t p$, acting in the *background* medium. However, the simplicity of Eqs. (1) and (2) is deceptive since the source terms on the right-hand side depend on the unknown *total* wave field quantities p and v_k inside D_{sct} . Nevertheless, if the scattered wave field is known on a surface surrounding the scatterer, ∂D_{sct} , then Eqs. (1) and (2) constitute an acoustic radiation problem and we have the following representation for the scattered pressure at any point, \mathbf{x}^R , outside D_{sct} (Fokkema and van den Berg, 1993):

$$p^{\text{sct}}(\mathbf{x}^R, \tau) = \int_0^{\tau} \int_{\partial D_{\text{sct}}} \left[G^q(\mathbf{x}^R | \mathbf{x}, \tau - t) v_k^{\text{sct}}(\mathbf{x}, t) + \Gamma_k^q(\mathbf{x}^R | \mathbf{x}, \tau - t) p^{\text{sct}}(\mathbf{x}, t) \right] n_k dA dt, \quad (3)$$

where $G^q(\mathbf{x}^R|\mathbf{x}, \tau - t)$ and $\Gamma_k^q(\mathbf{x}^R|\mathbf{x}, \tau - t)$ are the Green's functions for pressure and particle motion due to point sources of volume injection (q in the notation of Fokkema and van den Berg, 1993), respectively, in the *background* medium, ∂D_{sct} is the boundary of D_{sct} , and n_k are the components of the normal to the boundary.

Ting and Miksis (1986) have shown how Eq. (3) can be used to predict outgoing waves arriving at the boundary of a computational domain by extrapolating through free space the scattered wave field from an auxiliary surface surrounding the scatterer to the boundary. This involves substituting free-space Green's functions and evaluating Eq. (3) at time-retarded values t-r/c (with r=distance, c=wave speed, and r/c the travel time between the extrapolation surface and the boundary). Because the waves arriving at the edge of the computational domain are matched by the extrapolated waves, the boundary is nonreflecting.

3. Exact boundary conditions for perturbed scattering problems

If the scatterer occupies just a small part of the background model and the medium is inhomogeneous outside the extrapolation surface, ingoing waves resulting from interaction with the background model will be present and the above-presented approach no longer yields the correct boundary data required to truncate the computational domain. However, Eq. (3) may still be used to extrapolate the wave field to any point outside the extrapolation surface, as long as the exact, full wave form Green's functions for the inhomogeneous background model are used instead of free-space Green's functions. Multiple scattering between the perturbed region and the inhomogeneous background model of the radiated wave field may then affect the boundary data at all later times. We write Eq. (3) recursively to make the contribution of the scattered wave field at time *t* to all later times explicit. After discretizing the convolution integral in time this gives

$$\hat{p}^{\text{sct}}(\mathbf{x}^R, l, n) = \hat{p}^{\text{sct}}(\mathbf{x}^R, l, n - 1) + \int_{\partial D_{\text{sct}}} \left[\hat{G}^q(\mathbf{x}^R | \mathbf{x}, l - n) \hat{v}_k(\mathbf{x}, n) + \hat{\Gamma}_k^q(\mathbf{x}^R | \mathbf{x}, l - n) \hat{p}(\mathbf{x}, n) \right] n_k dA,$$
(4)

where a caret is used to differentiate between continuous time and sampled quantities. Note that the integral over t in Eq. (3) is implicit in the recursion in Eq. (4) and that the discrete-time indices l and n correspond to τ and t, respectively. Thus, to update the scattered wave field

 $p^{\text{sct}}(\mathbf{x}^R, l, n-1)$ at \mathbf{x}^R at time step n of the computation for all future time steps l > n, one has to

scale the Green's functions $\overset{\wedge}{G^q}(\mathbf{x}^R|\mathbf{x},l-n)$ and $n_k\overset{\wedge}{\Gamma_k^q}(\mathbf{x}^R|\mathbf{x},l-n)$ by the current value of the nor-

mal component of particle velocity $n_k, v_k(\mathbf{x}n)$, and the pressure $p(\mathbf{x}, n)$ on the extrapolation surface, respectively, and add this to the previously computed values at \mathbf{x}^R . Equation (4) needs

to be complemented by the incident wave field $p^{\text{inc}}(\mathbf{x}^R, n)$ to give the total wave field at \mathbf{x}^R . The resulting boundary condition is exact and equivalent to the Neumann series solution to the scattering problem (Snieder, 2002): It includes all orders of interactions between the background model and the perturbations.

To implement a wave field simulation on a limited region, Eq. (4) is used to update the boundary condition at each point on the boundary of the truncated domain, using the scattered wave field emitted from the perturbed domain at each time step. As in the method of Ting and Miksis, outgoing waves are absorbed at the boundary, because they are matched by the boundary condition. However, Eq. (4) also generates the desired incoming waves from higher order interactions with the background model, which are subsequently radiated inwards into the subgrid as desired. We now show how to compute the Green's functions in Eq. (4) required for extrapolation efficiently.

4. Interferometry

In the interferometric method, waves at two receiver locations are correlated to find the Green's function between them (Weaver and Lobkis, 2001). Recently, it was shown that there is a strong link between interferometry and reciprocity. Consider the acoustic reciprocity theorem of the correlation type (Fokkema and van den Berg, 1993);

$$\int_{\mathbf{x}\in\partial D} \left[C_t \{ p^A, \nu_k^B \} + C_t \{ \nu_k^A, p^B \} \right] n_k dA = \int_{\mathbf{x}\in D} \left[C_t \{ f_k^A, \nu_k^B \} + C_t \{ p^A, q^B \} + C_t \{ \nu_k^A, f_k^B, \} \right] + C_t \{ q^A, p^B \} dV, \tag{5}$$

where $C_{k}\{\cdot\}$ denotes temporal cross correlation. An interferometric representation for the pressure due to a point source of volume injection, $G^{q}(\mathbf{x}^{A}|\mathbf{x}^{B},t)$, between points \mathbf{x}^{A} and \mathbf{x}^{B} , can be derived by taking as state A the wave field generated by a point source of volume injection at \mathbf{x}^{A} : $\{p^{A}, v_{k}^{A}\}(\mathbf{x},t) = \{G^{q}, \Gamma_{k}^{q}\}(\mathbf{x}|\mathbf{x}^{A},t) \text{ and } \{q^{A}, f_{k}^{A}\}(\mathbf{x},t) = \{\delta(t)\delta(\mathbf{x}-\mathbf{x}^{A}),0\} \text{ and state } B \text{ the wave field generated by a point source of volume injection at } \mathbf{x}^{B}$: $\{p^{B}, v_{k}^{B}\}(\mathbf{x},t) = \{G^{q}, \Gamma_{k}^{q}\}(\mathbf{x}|\mathbf{x}^{B},t) \text{ and } \{q^{B}, f_{k}^{B}\}(\mathbf{x},t) = \{\delta(t)\delta(\mathbf{x}-\mathbf{x}^{B}),0\}.$

Inserting these expressions into Eq. (5), performing the volume integrations, and using reciprocity $[G^q(\mathbf{x}^A|\mathbf{x}^B,t)=G^q(\mathbf{x}^B|\mathbf{x}^A,t)]$ and $\Gamma_k^q(\mathbf{x}|\mathbf{x}^B,t)=-G_k^f(\mathbf{x}^B|x,t)]$ we find:

$$G^{q}(\mathbf{x}^{B}|\mathbf{x}^{A},t) + G^{q}(\mathbf{x}^{B}|\mathbf{x}^{A},-t) = -\int_{\mathbf{x}\in\partial D} \left[G^{q}(\mathbf{x}^{A}|\mathbf{x},t) * G_{k}^{f}(\mathbf{x}^{B}|\mathbf{x},-t) + G_{k}^{f}(\mathbf{x}^{A}|\mathbf{x},t) * G^{q}(\mathbf{x}^{B}|\mathbf{x},-t) \right] n_{k} dA,$$

$$(6)$$

where as asterisk denotes temporal convolution and $G_k^f(\mathbf{x}^B|x,t)$ denotes the pressure in \mathbf{x}^B due to a unidirectional point source force in the k direction at \mathbf{x} . Similarly, an interferometric representation for the pressure due to a point force source can be derived. By systematically illuminating a model from the surrounding surface, while storing the wave field in as many points in the interior as possible, full wave form Green's functions can be computed for any pair of points using only cross correlation and numerical integration (van Manen et al., 2005; 2006). This allows the Green's functions required to update the boundary condition to be computed efficiently and flexibly for any subdomain, once the initial illumination has been stored everywhere.

5. One-dimensional example

The exact boundary condition is demonstrated in an example using a staggered finite-difference approximation of the one-dimensional acoustic wave equation. The model consists of a single scattering layer (propagation velocity c_s =1750 m/s, mass density ρ_s =1250 kg/m³) embedded in a homogeneous background medium between 130 m and 170 m depth (c_0 =2000 m/s, ρ_0 =1000 kg/m³) and with a free surface at the top.

Since the model is one dimensional and bounded by a free surface at the top, a single source at the bottom of the well is sufficient to illuminate the model completely. Thus, only two conventional forward modeling runs were performed (one for each source type) and the data stored at every gridpoint. Nonreflecting boundary conditions were used just below the source to truncate the computational domain. Given the data of these two initial simulations, Green's functions between arbitrary points in the well can be computed using Eq. (6).

An incident wave field was calculated using interferometry, for a volume injection source at 50 m depth, and receivers collocated with the pressure points at the edge of the planned truncated computational domain. Since the finite-difference calculations are done on a staggered grid, whereas the Kirchhoff integral (and also the integral in the interferometric construction) is evaluated for the pressure and particle velocity quantities collocated in space and time, care should be taken that the required pressure and particle velocities are linearly interpolated to the same location and time.

Auxiliary extrapolation "surfaces" were defined just above and below the perturbation at 125 and 175 m depth, corresponding to boundary S in Fig. 1. Next, the model was significantly perturbed by increasing the velocity by 500 m/s and the density by 250 kg/m³ (both changes greater than 25%) in the scatterer. Since there is a free surface, waves scattering off the perturbation will reflect at the free surface and repeatedly interact with the perturbation. Thus, high-order, long-range interactions will be present, ruling out a Born approximation or conventional finite-difference injection to compute the response on the perturbed model.

To compute the response using the new methodology, the computational domain was truncated 15 m above and below the extrapolation points (at 110 and 190 m depth, respectively) corresponding to boundary *B* in Fig. 1. The offset of 15 m between the extrapolation surface and the boundary of the truncated domain was chosen to prevent errors due to the diffraction limit inherent in the interferometric Green's functions (de Rosny and Fink, 2002). Without loss of generality, we opted for a pressure (Dirichlet) boundary condition at the edge of the truncated computational domain and collocated the evaluation points of the Kirchhoff integral with the (staggered) *FD* pressure points at the edge of the grid. Thus, Green's functions for extrapolation through the background model need to be computed between all combinations of points with one point on the extrapolation and one point on the "injection" surface (i.e., between 125 and 110 m, 125 and 190 m, 175 and 110 m, and 175 and 190 m) and for both pressure-to-pressure and particle velocity-to-pressure interactions, giving a total of eight extrapolation Green's functions for this simple one-dimensional example.

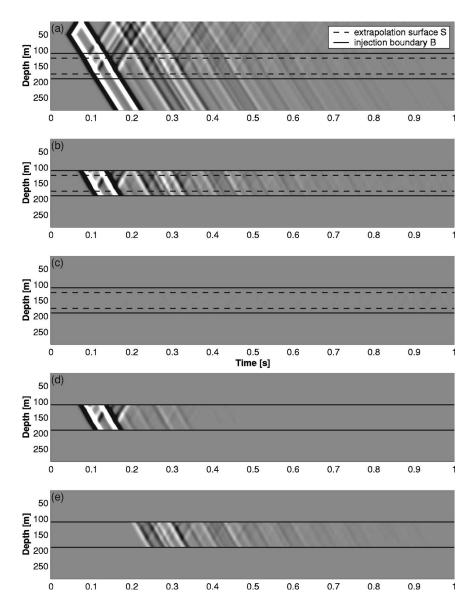


Fig. 2. Comparison of the proposed exact boundary condition and conventional FD injection to a directly computed reference. (a) Pressure, directly computed for the perturbed model by FD on the full grid. (b) Pressure, computed using the new method on the subgrid D. (c) Difference between (a) and (b) for the extent of the subgrid D, computed using conventional D injection. (e) Difference between (a) and (d) for the extent of the subgrid D, computed using conventional D injection.

In practice, the Kirchhoff extrapolation is evaluated for every time step of the finite-difference simulation on the truncated perturbed domain and the resulting seismograms used to update the buffer of future boundary values [Eq. (4)]. The next sample from the buffer is then used as the BC for the subsequent time step in the FD calculation. The wave field on the perturbed grid resulting from the new boundary condition is shown in Fig. 2(b). Note that no additional absorbing boundary conditions were used outside the new exact boundary condition. The resulting pressure wave field can be compared to a reference wave field in Fig. 2(a) calculated by a full FD simulation across the entire domain. In Fig. 2(c), the difference between Figs.

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2(a) and 2(b) is shown. The first high-order long-range interactions start between 0.2 and 0.24 s (depending on the depth). Thus, the high-order long-range interactions are reproduced exactly.

The main advance embodied in this method is to include all high-order, long-range interactions between the scattered wave field and the background medium. We therefore compare the results in Figs. 2(b) and 2(c) with corresponding results using the wave field injection method of Robertsson and Chapman (2002), shown in Figs. 2(d) and 2(e). That method only includes first-order, long-range interactions and hence, while the wave field simulated on the subdomain matches well at times up to 0.2 s, the arrival of the first, higher-order interaction thereafter causes errors in the local simulation. These are the errors that are removed by the new method.

6. Conclusion

The presented boundary condition is exact and can be used to compute the response, including all high-order, long-range interactions, to arbitrary perturbations in inhomogeneous models. There are no restrictions on the medium between the extrapolation surface and the boundary of the truncated computational domain as long as it is exactly the same as in the background model. No additional absorbing boundaries are necessary and no special functions need to be evaluated. It is possible to extend the method to cases where multiple, distinct subdomains of the model have been perturbed. In this case, the main result [Eq. (4)] is still valid but it should be used to update the boundary conditions at all boundary points around all subdomains at each time step, with wave fields extrapolated from boundary $\partial D_{\rm sct}$, which then spans the extrapolation surfaces of all subdomains. Thus, the presented approach also explicitly models the cross interactions between different finite-volume scattering regions. A key enabling feature of the new method is that the Green's functions required for extrapolation through the background model can be computed efficiently and flexibly using wave field interferometry. Finally, in principle the method can be extended to electromagnetic and elastic wave propagation.

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