

Generalized Waveform Inversion

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1 Introduction

In this document we derive the equations that are needed for developing a program that uses recorded waves to infer the properties of the material that is illuminated by a source. This can be an acoustic source - sound traveling through air or water, electro-magnetic source - light or radar, or elastic - sound waves traveling through solids. For sound traveling through air or fluids and for electro-magnetic phenomena the acoustic wave equation is used, for solids we will use the elastic wave equation. In particular we will derive the framework that is necessary for using domains: (i) formulate the equations for a domain that is bounded in space and (ii) linking the solution on the surface to the entire volume under investigation. There are three stages that we need to tackle to achieve a generalized approach.

1. acoustic: derive a domain decomposition approach that encapsulates both stiffness and density
2. elastic: derive the equations for elastic media, solving for Lamé parameters λ , μ and the density ρ .
3. detecting surfaces and imposing boundary conditions linking different media / discontinuities in the densities

The conjugent gradient scheme is particularly usefull for solving the smoothly varying properties throughout the medium. The objective of this research is to find a way to identify boundaries of different media as most information which is recorded is a result of those reflections. Also this is the most relevant information for interpreting the medium. Imaging techniques which reconstruct the field to obtain scattering information, although not very rigorously linked to the media properties, automatically make use of the strong scattering character of discontinuities in the velocity profile. Due to this and the computationally fast character of this approach it is still the main method used in seismology.

2 Wave Equation and Conservation Laws

2.1 Acoustic

2.2 Elastic

2.3 Coupling Two Media

3 From Data To Equations

3.1 Recorded Data in the Fourier Domain

4 Acoustic Wave Scattering

The objective of this section is to derive integral forms of the wave equations which will allow us to apply the conjugate gradient scheme to retrieve the media properties throughout space. Both stiffness $\kappa(\mathbf{r})$ and density $\rho(\mathbf{r})$ will be treated as unknowns of the physical system. An important part of the calculation will be to calculate the field given the updated media properties.

4.1 Representation theorem

Suppose we have 2 fields p_0 and p_1 which are obtained by illuminating the medium with properties $\kappa(\mathbf{r})$ and $\rho(\mathbf{r})$ by sources s_1 and s_2 respectively. They satisfy the following inhomogeneous differential equations

$$\frac{\omega^2}{\kappa} p_1 + \nabla \cdot \left(\frac{1}{\rho} \nabla p_1 \right) = -s_1 \quad (1)$$

$$\frac{\omega^2}{\kappa} p_2 + \nabla \cdot \left(\frac{1}{\rho} \nabla p_2 \right) = -s_2 \quad (2)$$

where we assume that the pressures and the forces vanish on the boundary as we take the boundary to infinity, i.e. the fields are L_2 integrable on \mathcal{R}^3 . We will subtract the second from the first equation after multiplying (1) by p_2 and (2) by p_1

$$\frac{\omega^2}{\kappa} p_1 p_2 + \nabla \cdot \left(\frac{1}{\rho} \nabla p_1 \right) p_2 = -s_1 p_2 \quad (3)$$

$$\frac{\omega^2}{\kappa} p_2 p_1 + \nabla \cdot \left(\frac{1}{\rho} \nabla p_2 \right) p_1 = -s_2 p_1 \quad (4)$$

Using the following identity

$$\nabla \cdot (f \mathbf{v}) = f \nabla \cdot \mathbf{v} + \nabla f \cdot \mathbf{v} \quad (5)$$

we can simplify the divergence terms

$$\nabla \cdot \left(p_2 \frac{1}{\rho} \nabla p_1 \right) = \nabla \cdot \left(\frac{1}{\rho} \nabla p_1 \right) p_2 + \frac{1}{\rho} \nabla p_1 \cdot \nabla p_2 \quad (6)$$

$$\nabla \cdot \left(p_1 \frac{1}{\rho} \nabla p_2 \right) = \nabla \cdot \left(\frac{1}{\rho} \nabla p_2 \right) p_1 + \frac{1}{\rho} \nabla p_2 \cdot \nabla p_1 \quad (7)$$

the last terms in equations (6) and (7) cancel when we subtract equation (2) from (1)

$$\nabla \cdot \left(\frac{1}{\rho} p_2 \nabla p_1 - \frac{1}{\rho} p_1 \nabla p_2 \right) = -(s_1 p_2 - s_2 p_1) \quad (8)$$

Integrating over volume V we obtain

$$\oint \left(\frac{1}{\rho} p_2 \nabla p_1 - \frac{1}{\rho} p_1 \nabla p_2 \right) \cdot \hat{\mathbf{n}} dS = - \int \{s_1 p_2 - s_2 p_1\} dV \quad (9)$$

where we've used Greens' identity to transform the volume integral over the divergent term into a surface integral.

Reciprocity

Representation theorem If we now take for p_1 the Greens function satisfying

$$\frac{\omega^2}{\kappa}G(\mathbf{r}, \mathbf{r}') + \nabla \cdot \left(\frac{1}{\rho} \nabla G(\mathbf{r}, \mathbf{r}') \right) = -\delta(\mathbf{r} - \mathbf{r}') \quad (10)$$

and for p_2 the field p and source term s then (9) becomes

$$p(\mathbf{r}) = \int s(\mathbf{r}')G(\mathbf{r}', \mathbf{r}) dV - \oint \frac{1}{\rho} \left(p(\mathbf{r}') \nabla G(\mathbf{r}', \mathbf{r}) - G(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS \quad (11)$$

When applied to a volume that doesn't contain sources the first term drops out and the representation theorem reduces to

$$p(\mathbf{r}) = \int s(\mathbf{r}')G(\mathbf{r}', \mathbf{r}) dV - \oint \frac{1}{\rho} \left(p(\mathbf{r}') \nabla G(\mathbf{r}', \mathbf{r}) - G(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS \quad (12)$$

which is known as the Kirchhoff equation for acoustic media.

4.2 Lippman-Schwinger Equation for Acoustic Media

In this section we derive an integral equation for the pressure field p of a general acoustic medium

$$L_A \circ p = \frac{\omega^2}{\kappa} p + \nabla \cdot \left(\frac{1}{\rho} \nabla p \right) = -s \quad (13)$$

The solution will be written in terms of a known field p_0 which satisfies a reference medium described by the differential operator $L_A^{(0)}$

$$L_A^{(0)} \circ p' = \frac{\omega^2}{\kappa_0} p' + \nabla \cdot \left(\frac{1}{\rho_0} \nabla p' \right) \quad (14)$$

p_0 is the field that the reference medium takes on under influence of source term s

$$L_A^{(0)} \circ p_0 = -s \quad (15)$$

The general operator can be written as the reference differential term plus a perturbed term

$$L_A = L_A^{(0)} + L_A^{(1)} \quad (16)$$

and the perturbed operator can now be calculated

$$L_A^{(1)} \circ p' = L_A - L_A^{(0)} = -\frac{\kappa_1}{\kappa_0} \frac{\omega^2}{\kappa} p' - \nabla \cdot \left(\frac{\rho_1}{\rho_0} \frac{1}{\rho} \nabla p' \right) \quad (17)$$

Here we've assumed that both the density as well as the stiffness can differ from the reference medium

$$\rho = \rho_0 + \rho_1 \quad (18)$$

$$\kappa = \kappa_0 + \kappa_1 \quad (19)$$

We introduce dimensionless fields to describe the density and stiffness perturbations

$$\chi_\rho = \frac{\rho_1}{\rho_0 + \rho_1} \quad \chi_\rho \in (-\infty, 1) \quad \rho_1 = \frac{\rho_0}{1 - \chi_\rho} \quad (20)$$

$$\chi_\kappa = \frac{\kappa_1}{\kappa_0 + \kappa_1} \quad \chi_\kappa \in (-\infty, 1) \quad \kappa_1 = \frac{\kappa_0}{1 - \chi_\kappa} \quad (21)$$

then the perturbation operator becomes

$$L_A^{(1)} \circ p' = -\frac{\omega^2}{\kappa_0} \chi_\kappa p' - \nabla \cdot \left(\frac{1}{\rho_0} \chi_\rho \nabla p' \right) \quad (22)$$

Scattering The equation of motion for the total field (13) can be written as satisfying the equation of motion for the reference media

$$L_A^{(0)} \circ p = -(s + L_A^{(1)} \circ p) \quad (23)$$

with source term $s_{\text{tot}} = s + L_A^{(1)} \circ p$ where $L_A^{(1)} \circ p$ can be interpreted as a virtual source term which depends on the field itself. We write the final solution as the sum of the reference field plus residual term

$$p = p_0 + p_1 \quad (24)$$

where we assume that p_0 satisfies

$$L_A^{(0)} \circ p_0 = -s \quad (25)$$

the solution to which we presumably know. Then for p_1 we can write

$$L_A^{(0)} \circ p_1 = -L_A^{(1)} \circ p \quad (26)$$

In literature p_1 is also known as the scattered field since it is the solution to the reference medium with the perturbation as its virtual source. We will make use of the representation theorem applied to the reference medium for which we need the Greens' function

$$L_A^{(0)} \circ G^{(0)}(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}') \quad (27)$$

which is also presumed to be known. The representation theorem for p_0 gives the identity

$$p_0(\mathbf{r}) = \int s(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV - \oint \left(\frac{1}{\rho_0} p_0(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - \frac{1}{\rho_0} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p_0(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS \quad (28)$$

in a volume without sources this expression reduces to

$$p_0(\mathbf{r}) = - \oint \left(\frac{1}{\rho_0} p_0(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - \frac{1}{\rho_0} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p_0(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS \quad (29)$$

This identity is the Kirchhoff integral and relates the field within a volume to the field values on its boundary.

The total field p can be written as the inhomogeneous solution to the unperturbed differential equation with source term $s_{\text{tot}} = s + L_A^{(1)} \circ p$. Then using the representation theorem with $G^{(0)}$ on equation (23)

$$p(\mathbf{r}) = \int_V s_{\text{tot}}(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' - \oint_S \frac{1}{\rho_0} \left\{ p(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right\} \cdot \hat{\mathbf{n}} dS' \quad (30)$$

Expanding s_{tot} and using the definition of $L_A^{(1)}$ we get

$$\begin{aligned} p(\mathbf{r}) &= \int_V s(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' \\ &\quad - \underbrace{\omega^2 \int \frac{1}{\kappa_0} \chi_\kappa p(\mathbf{r}') G^{(0)} dV - \int G^{(0)} \nabla \cdot \left(\frac{1}{\rho_0} \chi_\rho \nabla p(\mathbf{r}') \right) dV}_{I_\rho^{(V)}} \\ &\quad - \underbrace{\oint_S \frac{1}{\rho_0} \left(p(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) \right) \cdot \hat{\mathbf{n}} dS' + \oint_S \frac{1}{\rho_0} \left(G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS'}_{I_1^{(S)}} \end{aligned} \quad (31)$$

We can apply the div identity in equation (5) to the volume integral that corresponds to the density perturbation

$$I_\rho^{(V)} = - \int G^{(0)} \nabla \cdot \left(\frac{1}{\rho_0} \chi_\rho \nabla p \right) dV = \int \frac{1}{\rho_0} \chi_\rho \nabla G^{(0)} \cdot \nabla p dV - \underbrace{\oint \left(G^{(0)} \frac{1}{\rho_0} \chi_\rho \nabla p \right) \cdot \hat{\mathbf{n}} dS}_{I_2^{(S)}} \quad (32)$$

The surface integral $I_2^{(S)}$ in this expression can be combined with the surface integral $I_1^{(S)}$ from the expansion of $p(\mathbf{r})$ equation (31)

$$I_1^{(S)} + I_2^{(S)} = \oint_S \left(G^{(0)}(\mathbf{r}', \mathbf{r}) \left(\frac{1}{\rho_0} - \frac{1}{\rho_0} \chi_\rho \right) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS' \quad (33)$$

$$= \oint_S \left(\frac{1}{\rho} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS' \quad (34)$$

Putting these results back into equation (31) we arrive at the general Lippmann-Schwinger equation for acoustic wave scattering

$$\begin{aligned} p(\mathbf{r}) &= \int_V s(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' \\ &\quad - \omega^2 \int \frac{1}{\kappa_0} \chi_\kappa p(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' + \int \frac{1}{\rho_0} \chi_\rho \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) \cdot \nabla p(\mathbf{r}') dV' \\ &\quad - \oint_S \left(\frac{1}{\rho_0} p(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - \frac{1}{\rho} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS' \end{aligned} \quad (35)$$

This expression holds true for any source s , volume V , and general medium-reference medium pair characterized by $\{(\rho, \kappa), (\rho_0, \kappa_0)\}$.

4.3 Global Integral Equation

Here we adapt the integral equation for the case where we integrate over all of space. We rewrite the integral over sources using the representation theorem on the reference medium.

$$\int_V s(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' = p_0(\mathbf{r}) + \oint \frac{1}{\rho_0} \left(p_0 \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p_0 \right) \cdot \hat{\mathbf{n}} dS' \quad (36)$$

If we take a volume for which the fields and volumetric forces vanish on the boundary for the general and reference media, then the boundary conditions $G^{(0)}(\mathbf{r}', \mathbf{r}) = 0$ and $\nabla G^{(0)}(\mathbf{r}', \mathbf{r}) = 0$ for all $\mathbf{r}' \in S$ can be imposed on the integral equation (35) by eliminating the surface integrals. We obtain the global integral equation for p

$$p(\mathbf{r}) = p_0(\mathbf{r}) - \omega^2 \int_V \frac{1}{\kappa_0} \chi_\kappa p(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' + \int_V \frac{1}{\rho_0} \chi_\rho \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) \cdot \nabla p(\mathbf{r}') dV' \quad (37)$$

4.4 Local Integral Equation

When we focus on a particular area of space which doesn't contain any sources, v with boundary s , then the source term vanishes and the boundary integral persists.

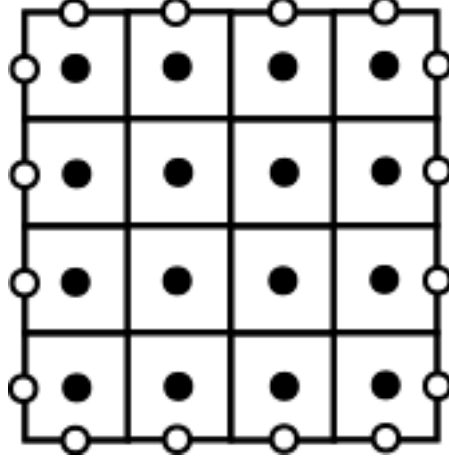
$$\begin{aligned} p(\mathbf{r}) = & -\omega^2 \int_v \frac{1}{\kappa_0} \chi_\kappa p(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV + \int_v \frac{1}{\rho_0} \chi_\rho \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) \cdot \nabla p(\mathbf{r}') dV \\ & - \oint_S \left(\frac{1}{\rho_0} p(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - \frac{1}{\rho} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS' \end{aligned} \quad (38)$$

Surface Integral Comparing the global scattering formula with the local version, one derives the following expression for the surface integral

$$- \oint_S \left(\frac{1}{\rho_0} p(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - \frac{1}{\rho} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS' \quad (39)$$

$$= p_0(\mathbf{r}) - \omega^2 \int_{\mathbf{r}' \notin v} \frac{1}{\kappa_0} \chi_\kappa p(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' + \int_{\mathbf{r}' \notin v} \frac{1}{\rho_0} \chi_\rho \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) \cdot \nabla p(\mathbf{r}') dV' \quad (40)$$

This equation tells us that the field on the surface of the domain contains all scattering information on the reference field and the direct illumination by the source. Note that for a perturbation which is 0 outside of v the surface integral equals $p_0(\mathbf{r})$.



5 Domain Decomposition

In this section we will define the discretized scheme that we use to numerically solve the wave equation. We will divide space of dimensions $L_x \times L_y \times L_z$ into $N_x \times N_y \times N_z$ hexahedron grid cells with sides $L_x/N_x, L_y/N_y, L_z/N_z$. Each domain consists of its interior v_i and boundary s_i which is explicitly modeled by separate elements.

The pressure field $p(\mathbf{r})$ is calculated iteratively through a series of fields $p^{(k)}(\mathbf{r})$, with $k = 0 \dots N_{it}$ and $p(\mathbf{r}) = \lim_{k \rightarrow \infty} p^{(k)}(\mathbf{r})$, which are evaluated at the reference points of the grid elements. The scheme is initiated by the unperturbed field

$$p^{(0)} = p_0$$

5.1 2D domains

Update Scheme for Velocity Variations In 2d we model the domain as depicted in diagram 5.1 where the reference points for interior grid cells are located at the cell mid-points and are represented by solid circles. The reference points for edges along the boundary s lie on their mid-points and are drawn as open circles.

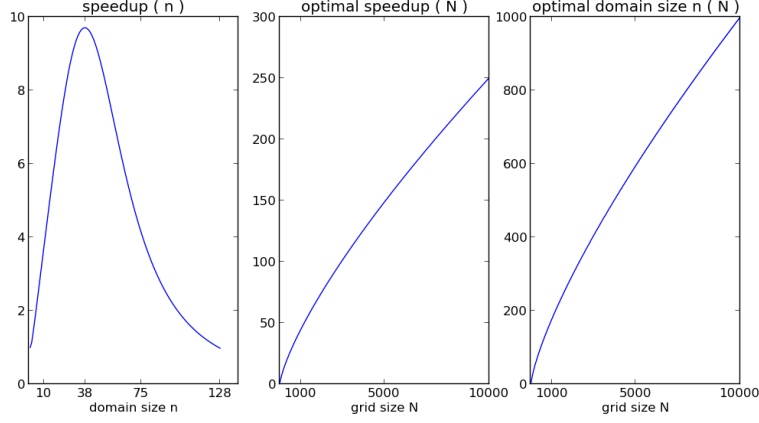
At this moment we will consider only variations in stiffness. Then we don't need to know the gradient of p for the interior elements of v . The update is done using the local version of the Lippmann-Swinger integral, equation (38), applied to the previous iteration

$$p_{\text{interior}}^{(k+1)}(\mathbf{r}) = -\omega^2 \int_v \frac{1}{\kappa_0} \chi_\kappa p^{(k)}(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV - \oint_s \left(\frac{1}{\rho_0} p^{(k)}(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) - \frac{1}{\rho_0} G^{(0)}(\mathbf{r}', \mathbf{r}) \nabla p^{(k)}(\mathbf{r}') \right) \cdot \hat{\mathbf{n}} dS' \quad (41)$$

The update for the boundary elements uses information of the full grid using equation (37)

$$p_{\text{boundary}}^{(k+1)}(\mathbf{r}) = p_0(\mathbf{r}) - \omega^2 \int_V \frac{1}{\kappa_0} \chi_\kappa p^{(k)}(\mathbf{r}') G^{(0)}(\mathbf{r}', \mathbf{r}) dV' \quad (42)$$

Figure 1: Speedup for full surface integration



The interior field, equation (41), needs the gradient of the pressure field on the boundary elements. To make the gradient for iteration k consistent with the field value $p_{\text{boundary}}^{(k)}$ we apply the gradient operator to equation (42)

$$\nabla p_{\text{boundary}}^{(k+1)}(\mathbf{r}) = \nabla p_0(\mathbf{r}) - \omega^2 \int_V \frac{1}{\kappa_0} \chi_{\kappa} p^{(k)}(\mathbf{r}') \nabla G^{(0)}(\mathbf{r}', \mathbf{r}) dV' \quad (43)$$

Update Scheme for Stiffness and Density Variations

5.2 3D domains

5.3 Speedup and Performance

The computational speedup for updating the surface of the domain by recalculating it using the whole grid is given by

$$\begin{aligned} s^{-1} &= \frac{1}{N^6} [(n^3)^2 + (n^3 - (n-1)^3) \cdot N^3] \cdot \frac{N^3}{n^3} \\ &= \frac{n^3}{N^3} + \frac{n^3 - (n-1)^3}{n^3} \\ &= \alpha + \beta \end{aligned} \quad (44)$$

where α is the relative volume occupied by the domain and β is the ratio of points on the boundary of the domain divided by the total number of blocks in the domain. α increases with n whereas β decreases with larger block volume. The optimum for a given size of the grid N can be obtained by solving $\partial_n \alpha + \partial_n \beta = 0$, for which one yields

$$\frac{(n-1)^2}{n^3} = \frac{n^3}{N^3} \quad (45)$$

In figure 1 the speedup as a function of domain size n is illustrated for $N = 128$. Also optimal speedups and domain sizes are plotted as a function of grid size N . The asymptotic behavior of the algorithmic speedup is given by

$$\alpha^{-1} \rightarrow N^{9/4} b l a$$

6 Path Integral Formulation

6.1 Acoustic path integral

6.2 Surface Variations

7 Elastic Wave Scattering

8 Fluid-solid interface