A Level Set-Adjoint State Method for the Joint Transmission-Reflection First-Arrival Traveltime Tomography with Unknown Reflector Position

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Abstract

We propose an efficient partial differential equation (PDE) based approach to the joint transmissionreflection traveltime tomography using first arrivals. In particular, we consider only the first arrivals from the transmission and reflection measurements at a series of receiver-source pairs. Unlike typical reflection tomography where the location of the reflector is assumed to be known by some migration techniques, we propose an efficient numerical approach based on the adjoint state method and the PDE based local level set method to invert both the piecewise smooth velocity within the computational domain and the location of a codimension-one reflector. Since we are using only first arrivals for tomography, we might not be able to obtain a perfect illumination of the reflector because the relevant information might be carried by the later arrivals. In this work, we propose an easily computed quantity which can quantify the reliability of our reconstruction. Numerical examples in both two- and three-dimensions will be given to demonstrate the efficiency of the proposed approach.

1 Introduction

One major concern in seismic applications is to determine the internal velocity or slowness of a medium by inverting the traveltime of waves between point sources and receivers [3, 39, 40, 31, 47, 48, 50, 32, 44]. Such inverse problem is classified as traveltime tomography. Depending on the nature of the measured traveltime field, there are various approaches to the inverse problem. For example, [4] proposed an algorithm to invert the slowness in the domain using the first arrival transmission traveltime, and so the resulting inverse problem is called the transmission traveltime tomography. Since this important work, many extensions to the inverse problem have been developed in the geophysics community more or less depending on a similar idea [5].

A related, yet different, inverse problem is the reflection traveltime tomography which concentrates on the wave reflected by the discontinuity in the slowness [11, 12]. To handle multi-offset data where the receivers have multiple arrivals from a point source, [8] has proposed a Lagrangian framework for reflective tomography. The fundamental idea is still to minimize the least-squares mismatch between the calculated values and the measurements. Other Lagrangian formulations can be found in [21, 20, 45, 43, 7]. In these works, the numerical approaches are designed to recover only the slowness in the media, while the location of the reflector is assumed to be known or is approximately inverted through some other migration techniques. A recent review on the subject can be found in [42].

A significantly harder problem is to further relax the assumption that the location of the reflector is known. Since [23] which proposes an efficient approach to handle multi-parameter classes, one can easily simultaneously estimate various parameters in the velocity model from different types of measurements. [14, 51] has proposed ray tracing approaches for determining both the velocity distribution and reflector position using only reflection traveltime measurements. To improve the reconstruction results, [52] has proposed a multi-stage approach to successively regularize the geometry of the reflector. Some other recent approaches to the problem can be found in, for example, [30, 38, 18, 16, 53]. However, the reflector location in all these works is represented explicitly using a parametrization. As one perturbs its location to minimize the mismatch functional, the triangulation may self-intersect or the topology of the

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reflector may change if the reflector splits into multiple surfaces. This is numerically challenging since one has to perform numerical surgery to remove unwanted grids and reconnect the remaining mesh.

Moreover, note that all above methods rely on ray tracing techniques based on the Fermat's principle. A major drawback of these Lagrangian approaches to first-arrival transmission traveltime tomography is that one has to develop a natural numerical approach to figure out the first arrival ray from multiple arrivals [37]. Also, since the curved rays are traveled in the inhomogeneous medium, there could be shadow regions between point sources and receivers [49, 1, 2].

In [26] and [25, 27], we have proposed simple partial differential equation (PDE) based approaches to the transmission tomography using first arrivals and multiple arrivals, respectively, so one can avoid using the ray tracing method. For the forward problem in the first-arrival transmission tomography [26], we model the first-arrival traveltimes from point sources by using the eikonal equation, where the viscosity solution of the Hamilton-Jacobi equation guarantees the first arrival at all receiver locations from a single point source [9]; and we derive an adjoint state equation to compute the needed gradient. We refer interested readers to [10] for some theoretical analysis of the approach. A similar inverse problem has recently been considered in [24] where the solution is determined on a triangular mesh using the fast marching method.

In practice, however, most important velocity models are discontinuous in the crust and lithosphere. The above approach will not work well since to stabilize the gradient flow, we have regularized the descent direction by a Tikhonov method which relies on the L^2 norm. Such regularity in the solution is too strong for the application and will in general lead to a continuous inverted velocity. In a recent paper [28], we have successfully extended the previous work [26] on first-arrival transmission traveltime tomography by restricting the inverted slowness in the class of piecewise continuous functions. In particular, the discontinuity in the velocity is represented implicitly using the level set method [34, 41, 33]. A similar inverse problem has been proposed recently in [55] which also study transmission traveltime tomography with discontinuous velocity; however, the paper [55] assumes that both the inside and outside slowness are **known**, which essentially reduces the inverse problem to a shape optimization problem.

Based on our previous works on transmission traveltime tomography on smooth velocity models [26] and piecewise smooth velocities [28], in this paper we first propose to develop an efficient PDE-based solver for joint transmission-reflection traveltime tomography using first arrivals. In particular, with given transmission and reflection first-arrivals traveltime measurements at a series of receiver-source pairs, we propose to invert **both** the piecewise smooth velocity within the computational domain and the location of a codimension-one reflector. The problem is significantly more challenging than typical transmission traveltime tomography or usual reflective traveltime tomography. Based on the level set method, the location of the reflector will be implicitly represented by the zero level set of a function defined over the whole domain. Its location will be adjusted accordingly using a gradient descent approach to minimize a least-squares type mismatch functional. To improve the computational efficiency, we apply the adjoint state method to also fit the piecewise smooth velocities in various subdomains separated by the unknown reflector. Another interesting application of the level set method in inverse problems can be found in [17].

An interesting recent paper [19] has also studied a joint transmission and reflection traveltime tomography problem. Identical to [26], the forward problem is modeled by the eikonal equation and is solved numerically using the fast sweeping method, while the variational derivative is also computed by the adjoint state equation which is in turn solved by the numerical method proposed in [26]. However, the location for the discontinuity in the model is still assumed to be **known** and one inverts the velocity only within certain sub-domain where the velocity is assumed to be continuous. The location of the discontinuity is not a part of their inverse problem.

Another contribution of the paper is a simple technique to quantify the confidence level of the inverted solution. Using only first arrivals for tomography, we might not be able to obtain a perfect illumination of the reflector since the information might be carried by the later arrivals. Instead of trying various extrapolation techniques, in this paper we propose an easily computed quantity which can be used to measure the reliability of our reconstruction.

The rest of the paper is organized as follows. In Section 2, we will introduce notations and will propose the problem statement for the paper. Based on the level set method and the adjoint state method, we propose a simple variational formula to invert both the unknown location of the reflector and the discontinuous velocity in Section 3. Regularization techniques will also be discussed in the section. To quantify the reliability in the inverted solutions, we propose a simple algorithm in Section 4. Section 5 summarizes the overall algorithm and gives detailed implementation strategies. Finally we will present numerical examples from both two- and three-dimensions in Section 6 to demonstrate the



Figure 1: Problem setup

effectiveness of the proposed algorithm.

2 Problem Statement

We study the seismic traveltime tomography in inhomogeneous media. The interface between different structures forms the reflector. As seismic wave hits these reflectors, reflection ray is generated. In this work, we will use these reflected waves together with the transmitted waves to investigate the media structure. We use the eikonal equation to formulate the nonlinear relationship between the traveltime and the media slowness. The inverse problem is to invert for the slowness distribution together with the reflector location using both first arrivals from the transmission and the reflection traveltime.

The setup is shown in figure 1. Let \mathbf{x}_s be the location of point source. In the case when there are more than one point source, we denote them with a superscript j, i.e. \mathbf{x}_s^j . R is the reflector which separates the regions Ω_1 and Ω_2 . We are interested in the slowness distribution $S(\mathbf{x})$ in the whole region $\overline{\Omega} = \overline{\Omega}_1 \cup \overline{\Omega}_2$. In this work we assume the slowness $S(\mathbf{x})$ is piecewise continuous, that is: $S(\mathbf{x}) = S_1(\mathbf{x})$, $\mathbf{x} \in \Omega_1$; $S(\mathbf{x}) = S_2(\mathbf{x})$, $\mathbf{x} \in \Omega_2$, and $S_1(\mathbf{x}) \in C(\Omega_1)$, $S_2(\mathbf{x}) \in C(\Omega_2)$.

The transmission traveltime $T_t(\mathbf{x})$ is given by the following eikonal equation,

$$|\nabla T_t(\mathbf{x})| = S(\mathbf{x}), \qquad \mathbf{x} \in \Omega \setminus \{\mathbf{x}_s\}$$
(1)

$$T_t(\mathbf{x}) = 0, \qquad \mathbf{x} = \mathbf{x}_s; \tag{2}$$

while the reflection traveltime $T_r(\mathbf{x})$ is calculated by

$$|\nabla T_r(\mathbf{x})| = S(\mathbf{x}), \qquad \mathbf{x} \in \Omega_1 \tag{3}$$

$$T_r(\mathbf{x}) = T_t(\mathbf{x}), \qquad \mathbf{x} \text{ on } R.$$
 (4)

We have receivers on Γ_2 to record the transmission traveltime T_t and receivers on Γ_1 to record the reflection traveltime T_r . The tomography problem reads as the following: given $T_t(\mathbf{x})$ on Γ_2 , $T_r(\mathbf{x})$ on Γ_1 , and the location of point sources $\mathbf{x}_s \in \Omega$, one inverts for the slowness distribution $S(\mathbf{x})$ and the location of the reflector R.

3 The level set adjoint state method

In this section, we apply the level set adjoint state method [28] to solve this tomography problem. The adjoint state method formulates the inverse problem as the minimization of a mismatch energy under constraint of the partial differential equation, and it evaluates the gradient of the mismatch energy by solving a system of adjoint equations.

In our problem, the mismatch energy is given by

$$E(S) = \frac{1}{2} \int_{\Gamma_1} |T_r - T_r^*|^2 \,\mathrm{d}s + \frac{1}{2} \int_{\Gamma_2} |T_t - T_t^*|^2 \,\mathrm{d}s\,, \tag{5}$$

where T_t^* corresponds to the first arrival traveltime of the transmission waves measured on Γ_2 , T_r^* is the first arrival traveltime of the reflection wave measured on Γ_1 . T_t and T_r are the corresponding viscosity solutions of equations (1), (2) and equations (3), (4), respectively. Our goal is to minimize this energy to find a suitable slowness $S(\mathbf{x})$. We mention that different from the tomography using only transmission traveltime, the reflection part in the joint tomography should be carefully treated.

3.1 Level set expression and perturbation of the slowness

Since we are concerned with a piecewise continuous slowness separated by a reflector, we use a level set function to express such structure:

$$S(\mathbf{x}) = S_1(\mathbf{x}) \cdot (1 - H(\phi(\mathbf{x}))) + S_2(\mathbf{x}) \cdot H(\phi(\mathbf{x})).$$

Here the level set function $\phi(\mathbf{x})$ is the signed distance to the reflector R,

$$\phi(\mathbf{x}) = \begin{cases} -\operatorname{dist}(\mathbf{x}, R) &, \quad \mathbf{x} \in \Omega_1 \\ \operatorname{dist}(\mathbf{x}, R) &, \quad \mathbf{x} \in \Omega_2 \end{cases}$$

and $H: \mathbb{R} \to \mathbb{R}$ is the Heaviside function with

$$H(x) = \begin{cases} 0 & , x < 0 \\ 1 & , x > 0 \end{cases}.$$

One inverts for the value of $\phi(\mathbf{x})$ to locate the reflector $R = \phi^{-1}(0)$ and the values of $S_1(\mathbf{x})$ and $S_2(\mathbf{x})$ to obtain the slowness distribution. In an iterative algorithm, one starts from an initial guess and perturbs these parameters step by step. To study the dependence of $S(\mathbf{x})$ on the perturbations of $\phi(\mathbf{x})$, $S_1(\mathbf{x})$ and $S_2(\mathbf{x})$, we use a smoothed version of the Heaviside function by introducing a small parameter τ ($0 < \tau < 1$),

$$H_{\tau}(\phi) = \frac{1}{2} \left(\tanh \frac{\phi}{\tau} + 1 \right).$$
(6)

Then the slowness is expressed as

$$S(\mathbf{x}) = S_1(\mathbf{x}) \cdot (1 - H_\tau(\phi(\mathbf{x}))) + S_2(\mathbf{x}) \cdot H_\tau(\phi(\mathbf{x})),$$
(7)

and the perturbation is given by

$$S(\phi + \epsilon \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - S(\phi, S_1, S_2) = (S_2 - S_1) \cdot (H_\tau(\phi + \epsilon \tilde{\phi}) - H_\tau(\phi)) + \epsilon \tilde{S}_1 \cdot (1 - H_\tau(\phi + \epsilon \tilde{\phi})) + \epsilon \tilde{S}_2 \cdot H_\tau(\phi + \epsilon \tilde{\phi}).$$
(8)

We evaluate the perturbation of the Heaviside function as in our previous work on transmission tomography [28]. One can refer to formulas (6-8) in that article and here we simply state the results,

$$H_{\tau}(\phi + \epsilon \tilde{\phi}) - H_{\tau}(\phi) = \epsilon \tilde{\phi} \cdot \frac{1}{2\tau \cdot \cosh^2 \frac{\phi}{\tau}} - \epsilon^2 \tilde{\phi}^2 \cdot \frac{\tanh \frac{\xi}{\tau}}{2\tau^2 \cdot \cosh^2 \frac{\xi}{\tau}} \\ = \begin{cases} O(1) &, \quad \phi = O(\tau^{\alpha}) \text{ and } \alpha \ge 1\\ O(\epsilon) &, \quad \phi = O(\tau^{\alpha}) \text{ and } \alpha < 1 \end{cases},$$
(9)

where $\xi \in (\phi, \phi + \epsilon \tilde{\phi})$ and the notation f = O(g) means $\exists C > 0$, such that $|f| \leq C|g|$. The order is estimated in the sense of $\tau \to 0$, and we choose $\epsilon \leq \tau$. Again note that $\phi = O(\tau^{\alpha})$ where $\alpha \geq 1$ only near the reflector R, thus in the limit as $\tau \to 0$ such region is of zero measure. Plugging the evaluation (9) into (8), we get

$$S(\phi + \epsilon \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - S(\phi, S_1, S_2) = \begin{cases} O(1) & , \quad \phi = O(\tau^{\alpha}) \text{ and } \alpha \ge 1\\ O(\epsilon) & , \quad \phi = O(\tau^{\alpha}) \text{ and } \alpha < 1 \end{cases}$$
(10)

In the following we derive the corresponding change in the arrival time T_t and T_r due to the perturbation of the slowness $S(\mathbf{x})$, denoted by δT_t and δT_r .

The transmission arrival time $T_t(\mathbf{x})$ depends on the accumulation of the slowness along the ray reaching \mathbf{x} . Similar to the argument in our previous work [28], we look at

$$T_t(\mathbf{x}) = \int_0^L S(s) ds = \int_{[0,L] \cap \{\phi = O(\tau^{\alpha}), \ \alpha \ge 1\}} S(s) ds + \int_{[0,L] \cap \{\phi = O(\tau^{\alpha}), \ \alpha < 1\}} S(s) ds$$
(11)

where S(s) corresponds to the arc-length parametrization of the ray s from the point source to the point **x**. Note that this is a very nonlinear problem because L depends on S implicitly. Since the measure of the set $\{\phi = O(\tau^{\alpha}), \alpha \geq 1\}$ is $O(\tau) = O(\epsilon)$, we expect the corresponding change of $T_t(\mathbf{x})$ due to the perturbation in (10) is of $O(\epsilon)$, viz. $\delta T_t = O(\epsilon)$.

The perturbation on the reflection travel time $T_r(\mathbf{x})$ is unfortunately slightly more complicated. Looking at (3) and (4), one finds that several parameters affect the solution $T_r(\mathbf{x})$, including the domain Ω_1 , the slowness distribution $S(\mathbf{x})$ in Ω_1 , the location of the reflector R and the values of $T_t(\mathbf{x})$ on R. All these related parameters will be affected once we perturb $S(\phi, S_1, S_2)$ in (10), and the change of Ω_1 (and therefore the boundary location R) usually introduces abrupt changes to the solution $T_r(\mathbf{x})$. To obtain a smooth change in successive iterations, we first imagine that we perturb only S_1 and S_2 , while fixing ϕ to get $S(\phi, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2)$. Then the domain of $T_r(\mathbf{x})$, Ω_1 , and the boundary R are frozen, thus δT_r only relates to the perturbation of $S(\mathbf{x})$ in Ω_1 and the change of $T_t(\mathbf{x})$ on R. Since we already know that $\delta T_t(\mathbf{x}) = O(\epsilon)$ and the perturbation of $S(\mathbf{x})$ is depicted by (10), using the same argument as for $T_t(\mathbf{x})$ we can expect that the corresponding perturbation on $T_r(\mathbf{x})$ is of $O(\epsilon)$. In practice of course we cannot have ϕ frozen since we have to invert for the location of the reflector, while the above consideration inspires us that we can reduce the perturbation on ϕ to control the magnitude of δT_r . Therefore we introduce a small parameter ν ($0 < \nu < 1$) to $\tilde{\phi}$ and use $\nu \tilde{\phi}$ as the perturbation in the level set function. And so with $\delta S = S(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - S(\phi, S_1, S_2)$, we expect that the change in Ω_1 (and so the change in R) is very small. Thus the relation $\delta T_r(\mathbf{x}) = O(\epsilon)$ holds almost everywhere in Ω_1 .

In summary, with the perturbation of the slowness

$$\delta S = S(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - S(\phi, S_1, S_2), \qquad (12)$$

we expect the corresponding perturbation on the traveltime is in the form of

$$T_t(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - T_t(\phi, S_1, S_2) = \epsilon \cdot \tilde{T}_t \qquad a.e. \text{ in } \Omega$$
(13)

$$T_r(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - T_r(\phi, S_1, S_2) = \epsilon \cdot \tilde{T}_r \qquad a.e. \text{ in } \Omega_1, \tag{14}$$

where a.e. denotes almost everywhere.

Then combining (13) and (14) with the eikonal equation (1), we can derive the formulas directly relating $\tilde{\phi}$, \tilde{S}_1 , \tilde{S}_2 , \tilde{T}_t and \tilde{T}_r . This derivation is standard as in our previous work on transmission tomography [28], we put the detailed calculation in Appendix A and here we write down the results:

$$\nu \tilde{\phi} \cdot A(\phi, S_1, S_2) + \tilde{S}_1 \cdot B(\phi, S_1, S_2) + \tilde{S}_2 \cdot C(\phi, S_1, S_2) - \nabla T_t \cdot \nabla \tilde{T}_t = 0,$$
(15)

$$\nu \tilde{\phi} \cdot A(\phi, S_1, S_2) + \tilde{S}_1 \cdot B(\phi, S_1, S_2) + \tilde{S}_2 \cdot C(\phi, S_1, S_2) - \nabla T_r \cdot \nabla \tilde{T}_r = 0,$$
(16)

where the notations A, B and C denote

$$A(\phi, S_1, S_2) = S(\phi, S_1, S_2) \cdot \frac{S_2 - S_1}{2\tau \cdot \cosh^2 \frac{\phi}{\pi}},$$
(17)

$$B(\phi, S_1, S_2) = S(\phi, S_1, S_2) \cdot (1 - H_\tau(\phi)), \qquad (18)$$

$$C(\phi, S_1, S_2) = S(\phi, S_1, S_2) \cdot H_{\tau}(\phi).$$
(19)

Note that (15) is valid *a.e.* in Ω and (16) is valid *a.e.* in Ω_1 .

3.2 Adjoint state method for the gradient

Now we use the adjoint state method to calculate the gradient-descent direction of the mismatch energy. With (5), (13) and (14), the perturbation on the mismatch energy is given by

$$\delta E/\epsilon = [E(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - E(\phi, S_1, S_2)]/\epsilon$$

$$= \int_{\Gamma_1} \tilde{T}_r (T_r - T_r^*) \mathrm{d}s + \int_{\Gamma_2} \tilde{T}_t (T_t - T_t^*) \mathrm{d}s + O(\epsilon).$$
(20)

Our purpose is to remove the dependence of \tilde{T}_t and \tilde{T}_r in (20) by introducing adjoint state equations. To simplify the notation, we denote

$$W = \nu \tilde{\phi} \cdot A(\phi, S_1, S_2) + \tilde{S}_1 \cdot B(\phi, S_1, S_2) + \tilde{S}_2 \cdot C(\phi, S_1, S_2),$$
(21)

where A, B and C are given by (17-19). And we have the following results.

Lemma 3.1. If λ satisfies the adjoint state equation

$$-div(\lambda \nabla T_t) = 0, \qquad in \ \Omega \tag{22}$$

$$\lambda \frac{\partial I_t}{\partial \mathbf{n}} = T_t - T_t^*, \quad on \ \Gamma_2 \tag{23}$$

$$\lambda = 0, \qquad on \ \partial\Omega \setminus \Gamma_2, \tag{24}$$

where **n** denotes the unit outward normal of $\partial \Omega$, then (20) can be reduced to

 \mathbf{n}

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W d\mathbf{x} + \int_{\Gamma_1} \tilde{T}_r (T_r - T_r^*) ds + O(\epsilon)$$
(25)

and so the dependence of \tilde{T}_t is removed.

Lemma 3.2. If μ satisfies the adjoint state equation

$$-\operatorname{div}(\mu\nabla T_r) = 0, \qquad \operatorname{in}\,\Omega_1 \tag{26}$$

$$\mu \frac{\partial T_r}{\partial \mathbf{n}} = T_r - T_r^*, \qquad on \ \Gamma_1 \tag{27}$$

$$\mu = 0, \qquad on \ \partial\Omega_1 \setminus (R \cup \Gamma_1), \tag{28}$$

and $\hat{\mu}$ satisfies the adjoint state equation

$$-div(\hat{\mu}\nabla T_t) = 0, \qquad in \ \Omega_1 \tag{29}$$

$$\hat{\mu} = \mu, \qquad on \ R \tag{30}$$

$$\hat{\mu} = 0, \qquad on \ \partial\Omega_1 \setminus R,$$
(31)

the perturbation of the mismatch energy can be further reduced to

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W d\mathbf{x} + \int_{\Omega_1} (\mu + \hat{\mu}) W d\mathbf{x} + O(\epsilon) \,. \tag{32}$$

Thus the dependence of \tilde{T}_r is also removed.

We put the detailed derivations of these two lemmas in Appendix B, the idea is to eliminate \tilde{T}_t and \tilde{T}_r in (20) using the formulas (15) and (16) which relate the perturbations of the slowness to the perturbations of the traveltime. We further mention that it is not straight-forward to eliminate \tilde{T}_r since one has to maintain an inflow boundary condition for the adjoint state equation such that the boundary condition propagates from receivers back into the unknown interior region. For details, please refer to Appendix B.

Note that the adjoint state variables μ and $\hat{\mu}$ are defined only in Ω_1 . If necessary, we can extend them to the whole Ω simply by setting

$$\mu(\mathbf{x}) = \begin{cases} \mu(\mathbf{x}) &, \quad \mathbf{x} \in \Omega_1 \\ 0 &, \quad \mathbf{x} \in \Omega \setminus \Omega_1 \end{cases}$$
(33)

and

$$\hat{\mu}(\mathbf{x}) = \begin{cases} \hat{\mu}(\mathbf{x}) &, \quad \mathbf{x} \in \Omega_1 \\ 0 &, \quad \mathbf{x} \in \Omega \setminus \Omega_1 \end{cases}$$
(34)

Thus (32) can be rewritten as

$$\frac{\delta E}{\epsilon} = \int_{\Omega} (\lambda + \mu + \hat{\mu}) W \,\mathrm{d}\mathbf{x} + O(\epsilon). \tag{35}$$

Using formula (21) and neglecting the $O(\epsilon)$ term in (35), we obtain the descent direction of the perturbation when

$$\tilde{\phi} = -A(\phi, S_1, S_2) \cdot (\lambda + \mu + \hat{\mu}), \qquad (36)$$

$$S_1 = -B(\phi, S_1, S_2) \cdot (\lambda + \mu + \hat{\mu}), \tag{37}$$

$$\hat{S}_2 = -C(\phi, S_1, S_2) \cdot (\lambda + \mu + \hat{\mu});$$
(38)

where A, B and C are given by (17-19). With these perturbations chosen in this particular way, we have

$$\delta E \approx -\epsilon \cdot \int_{\Omega} (\lambda + \mu + \hat{\mu})^2 \left(\nu A^2 + B^2 + C^2\right) \mathrm{d}\mathbf{x} \le 0.$$

3.3 Regularizations of $\phi(\mathbf{x})$, $S_1(\mathbf{x})$ and $S_2(\mathbf{x})$

In previous subsections, we have introduced the level set adjoint state method for the transmissionreflection tomography problem where we invert for the level set function $\phi(\mathbf{x})$ and the slowness functions $S_1(\mathbf{x})$ and $S_2(\mathbf{x})$ on both sides of the reflector. Since the inverse problem is highly ill-posed, it is necessary to impose regularizations on these parameters.

For the level set function $\phi(\mathbf{x})$, we use the level set re-initialization to maintain ϕ as a signed distance function. This is the same as the treatment in our previous work of transmission tomography [28]. Specifically we solve the following system in an artificial time direction ξ

$$\frac{\partial \Phi}{\partial \xi} + \operatorname{sign}(\phi) \cdot (|\nabla \Phi| - 1) = 0, \tag{39}$$

$$\left. \frac{\partial \Phi}{\partial \mathbf{n}} \right|_{\partial \Omega} = 0, \tag{40}$$

with the initial condition $\Phi|_{\xi=0} = \phi$ and $\operatorname{sign}(\phi) = \frac{2}{\pi} \arctan \phi$ is the signum function [33]. Since we are only interested in the solution near the zero level set, in practice there is no need to get the steady state solution. Solving the system for several $\Delta \xi$ steps (in our implementation usually 6 steps), we finally update the original level set function using the intermediate solution Φ .

Also, as we mentioned in subsection 3.1, the reflection ray is very sensitive to the perturbation of ϕ since ϕ is used to describe the location of the reflector R. To maintain a stable iteration we reduce such sensitivity by imposing an extra regularization to smoothen the shape of the reflector R. And this is achieved by penalizing the L^2 norm of $\nabla \phi(\mathbf{x})$ which is added to our previous defined mismatch energy,

$$E_{\text{new}} = E + \gamma \cdot E_{\phi} \tag{41}$$

where E is given by formula (5), γ is a parameter to control the weight, and E_{ϕ} measures the L^2 norm of $\nabla \phi$ given by

$$E_{\phi} = \frac{1}{2} \int_{\Omega} |\nabla \phi|^2 \mathrm{d}\mathbf{x}.$$
(42)

When the slowness perturbation is given by (12), the corresponding change in E_{ϕ} is

$$\delta E_{\phi} = E_{\phi}(\phi + \epsilon \cdot \nu \tilde{\phi}) - E_{\phi}(\phi)$$

$$= \epsilon \nu \cdot \int_{\Omega} \nabla \phi \cdot \nabla \tilde{\phi} \, \mathrm{d}\mathbf{x} + O(\epsilon^{2})$$

$$= \epsilon \nu \cdot \left[-\int_{\Omega} \Delta \phi \cdot \tilde{\phi} \, \mathrm{d}\mathbf{x} + \int_{\partial \Omega} \frac{\partial \phi}{\partial \mathbf{n}} \cdot \tilde{\phi} \, \mathrm{d}s \right] + O(\epsilon^{2}).$$
(43)

In (43), $\phi(\mathbf{x})$ is the level set function before perturbation but after re-initialization. Since we have $\frac{\partial \phi}{\partial \mathbf{n}}\Big|_{\partial\Omega} = 0$ due to (40), (43) leads to

$$\delta E_{\phi} = -\epsilon \nu \cdot \int_{\Omega} \Delta \phi \cdot \tilde{\phi} \, \mathrm{d}\mathbf{x} + O(\epsilon^2) \,. \tag{44}$$

Combining (35), (41) and (44), we have

$$\frac{\delta E_{\text{new}}}{\epsilon} = \frac{\delta E}{\epsilon} + \gamma \cdot \frac{\delta E_{\phi}}{\epsilon}
= \int_{\Omega} \nu \tilde{\phi} \cdot \left[(\lambda + \mu + \hat{\mu}) A(\phi, S_1, S_2) - \gamma \Delta \phi \right] d\mathbf{x}
+ \int_{\Omega} (\lambda + \mu + \hat{\mu}) \cdot \left(\tilde{S}_1 \cdot B(\phi, S_1, S_2) + \tilde{S}_2 \cdot C(\phi, S_1, S_2) \right) d\mathbf{x} + O(\epsilon).$$
(45)

Thus to get the gradient descent of the newly defined mismatch energy E_{new} , the perturbation on ϕ should be modified as

$$\tilde{\phi} = -A(\phi, S_1, S_2) \cdot (\lambda + \mu + \hat{\mu}) + \gamma \Delta \phi,$$
(46)

where the term $\gamma \Delta \phi$ provides the regularization to control the shape of the reflector.

Next we provide the regularization for $S_1(\mathbf{x})$ and $S_2(\mathbf{x})$. Since we are interested in the piecewise continuous structure, we smooth their corresponding perturbations $\tilde{S}_1(\mathbf{x})$ and $\tilde{S}_2(\mathbf{x})$ at each iteration. With (45), the corresponding change of the mismatch energy due to \tilde{S}_1 is

$$\delta E_{S_1} := \epsilon \cdot \int_{\Omega} (\lambda + \mu + \hat{\mu}) B(\phi, S_1, S_2) \tilde{S}_1 \, \mathrm{d}\mathbf{x},\tag{47}$$

thus \tilde{S}_1 is selected as in (37) to achieve the gradient descent. Also the corresponding change of the mismatch energy due to \tilde{S}_2 is

$$\delta E_{S_2} := \epsilon \cdot \int_{\Omega} (\lambda + \mu + \hat{\mu}) C(\phi, S_1, S_2) \tilde{S}_2 \, \mathrm{d}\mathbf{x}, \tag{48}$$

and so \tilde{S}_2 is chosen to be the form in (38). We smooth \tilde{S}_1 and \tilde{S}_2 by solving the following equations,

$$(I - \alpha \Delta)\tilde{S}_{1}^{*} = \tilde{S}_{1} = -B(\phi, S_{1}, S_{2}) \cdot (\lambda + \mu + \hat{\mu}), \quad \text{in } \Omega$$
$$\frac{\partial \tilde{S}_{1}^{*}}{\partial \mathbf{n}} = 0, \quad \text{on } \partial\Omega$$
(49)

and

$$(I - \alpha \Delta)\tilde{S}_{2}^{*} = \tilde{S}_{2} = -C(\phi, S_{1}, S_{2}) \cdot (\lambda + \mu + \hat{\mu}), \quad \text{in } \Omega$$
$$\frac{\partial \tilde{S}_{2}^{*}}{\partial \mathbf{n}} = 0, \quad \text{on } \partial\Omega$$
(50)

where I is the identity operator, Δ is the Laplace operator and $\alpha > 0$ is the weight controlling the amount of regularity one wants. Then we use \tilde{S}_1^* and \tilde{S}_2^* to replace \tilde{S}_1 and \tilde{S}_2 in the perturbation, which leads to

$$\delta E_{S_1} = \epsilon \cdot \int_{\Omega} (\lambda + \mu + \hat{\mu}) B(\phi, S_1, S_2) \cdot \tilde{S}_1^* \, \mathrm{d}\mathbf{x}$$
$$= -\epsilon \cdot \int_{\Omega} (I - \alpha \Delta) \tilde{S}_1^* \cdot \tilde{S}_1^* \, \mathrm{d}\mathbf{x}$$
$$= -\epsilon \cdot \int_{\Omega} \left[\left(\tilde{S}_1^* \right)^2 + \alpha \left| \nabla \tilde{S}_1^* \right|^2 \right] \, \mathrm{d}\mathbf{x} \le 0$$

and

$$\delta E_{S_2} = -\epsilon \cdot \int_{\Omega} \left[\left(\tilde{S}_2^* \right)^2 + \alpha \left| \nabla \tilde{S}_2^* \right|^2 \right] \mathrm{d}\mathbf{x} \le 0.$$

3.4 Summary of formulas for multiple point sources

In above subsection, we provide the level set adjoint state method for the joint transmission-reflection traveltime tomography, where we deal with the data set of first-arrival traveltime $T_t^*|_{\Gamma_1}$ and $T_r^*|_{\Gamma_2}$ collected from the rays emanating from one single point source. In typical seismic survey, we perform such experiment many times and so we get multiple sets of data with each set corresponding to rays emanating from one of those multiple point sources. In this subsection, we summarize formulas to deal with the multiple data set.

Specifically we denote $T^*_{t,j}|_{\Gamma_1}$ and $T^*_{r,j}|_{\Gamma_2}$ the data sets corresponding to the point source located at \mathbf{x}^j_s , $j = 1, 2, 3, \dots, N$. We simply sum up all individual mismatch energy and minimize

$$E^{N}(\phi, S_{1}, S_{2}) = \frac{1}{2} \sum_{j=1}^{N} \int_{\Gamma_{1}} \left| T_{r,j} - T_{r,j}^{*} \right|^{2} \mathrm{d}s + \frac{1}{2} \sum_{j=1}^{N} \int_{\Gamma_{2}} \left| T_{t,j} - T_{t,j}^{*} \right|^{2} \mathrm{d}s + \gamma \cdot \frac{1}{2} \int_{\Omega} \left| \nabla \phi \right|^{2} \mathrm{d}\mathbf{x}, \tag{51}$$

where $T_{t,j}$ and $T_{r,j}$ are the solutions to (1-2) and (3-4) respectively, corresponding to the point source \mathbf{x}_s^j . With almost the same calculation as above, we have the perturbation of E^N ,

$$\frac{\delta E^{N}}{\epsilon} = \frac{E^{N}(\phi + \epsilon \nu \tilde{\phi}, S_{1} + \epsilon \tilde{S}_{1}, S_{2} + \epsilon \tilde{S}_{2}) - E^{N}(\phi, S_{1}, S_{2})}{\epsilon}$$

$$= \int_{\Omega} \nu \tilde{\phi} \cdot \left[\sum_{j} (\lambda_{j} + \mu_{j} + \hat{\mu}_{j}) A(\phi, S_{1}, S_{2}) - \gamma \Delta \phi \right] d\mathbf{x}$$

$$+ \int_{\Omega} \sum_{j} (\lambda_{j} + \mu_{j} + \hat{\mu}_{j}) \cdot \left(\tilde{S}_{1} \cdot B(\phi, S_{1}, S_{2}) + \tilde{S}_{2} \cdot C(\phi, S_{1}, S_{2}) \right) d\mathbf{x} + O(\epsilon) \quad (52)$$

where A, B and C are given by formulas (17), (18) and (19). Also the variables λ_j , μ_j and $\hat{\mu}_j$ are computed by solving the following adjoint state equations:

$$-\operatorname{div}(\lambda_{j} \nabla T_{t,j}) = 0, \quad \text{in } \Omega$$
$$\lambda_{j} \frac{\partial T_{t,j}}{\partial \mathbf{n}} = T_{t,j} - T_{t,j}^{*}, \quad \text{on } \Gamma_{2}$$
$$\lambda_{j} = 0, \quad \text{on } \partial\Omega \setminus \Gamma_{2}, \quad (53)$$

$$-\operatorname{div}(\mu_{j}\nabla T_{r,j}) = 0, \quad \text{in } \Omega_{1}$$

$$\mu_{j}\frac{\partial T_{r,j}}{\partial \mathbf{n}} = T_{r,j} - T_{r,j}^{*}, \quad \text{on } \Gamma_{1}$$

$$\mu_{j} = 0, \quad \text{on } \partial\Omega_{1} \setminus (R \cup \Gamma_{1}), \quad (54)$$

and

$$-\operatorname{div}(\hat{\mu}_{j} \nabla T_{t,j}) = 0, \quad \text{in } \Omega_{1}$$
$$\hat{\mu}_{j} = \mu_{j}, \quad \text{on } R$$
$$\hat{\mu}_{j} = 0, \quad \text{on } \partial \Omega_{1} \setminus R,$$
(55)

and we extend the values of μ_j and $\hat{\mu}_j$ to the whole domain Ω by simply setting

$$\mu_j = \begin{cases} \mu_j &, \text{ in } \Omega_1 \\ 0 &, \text{ in } \Omega \setminus \Omega_1 \end{cases}$$
(56)

$$\hat{\mu}_j = \begin{cases} \hat{\mu}_j &, & \text{in } \Omega_1 \\ 0 &, & \text{in } \Omega \setminus \Omega_1 \end{cases}$$
(57)

To achieve the gradient descent, $\tilde{\phi}$ is set to be

$$\tilde{\phi} = -\sum_{j} (\lambda_j + \mu_j + \hat{\mu}_j) \cdot A(\phi, S_1, S_2) + \gamma \Delta \phi , \qquad (58)$$

where \tilde{S}_1 and \tilde{S}_2 are obtained by solving the regularization equations:

$$(I - \alpha \Delta)\tilde{S}_1 = -B(\phi, S_1, S_2) \cdot \sum_j (\lambda_j + \mu_j + \hat{\mu}_j), \quad \text{in } \Omega$$
$$\frac{\partial \tilde{S}_1}{\partial \mathbf{n}} = 0, \quad \text{on } \partial \Omega$$
(59)

and

$$(I - \alpha \Delta)\tilde{S}_2 = -C(\phi, S_1, S_2) \cdot \sum_j (\lambda_j + \mu_j + \hat{\mu}_j), \quad \text{in } \Omega$$
$$\frac{\partial \tilde{S}_2}{\partial \mathbf{n}} = 0, \quad \text{on } \partial\Omega.$$
(60)

Then the parameters $\phi(\mathbf{x})$, $S_1(\mathbf{x})$ and $S_2(\mathbf{x})$ are updated by

$$\begin{split} \phi^{\text{new}}(\mathbf{x}) &= \phi^{\text{old}}(\mathbf{x}) + \epsilon \cdot \nu \tilde{\phi}, \\ S_1^{\text{new}}(\mathbf{x}) &= S_1^{\text{old}}(\mathbf{x}) + \epsilon \cdot \tilde{S}_1, \\ S_2^{\text{new}}(\mathbf{x}) &= S_2^{\text{old}}(\mathbf{x}) + \epsilon \cdot \tilde{S}_2. \end{split}$$

Finally, we re-initialize the level set function $\phi(\mathbf{x})$ by solving (39-40) and then update the slowness distribution $S(\mathbf{x})$ using formula (7).

4 Indication of unilluminated regions

In this section, we study the reliability of our reconstruction. It is common in seismic tomography that there are shadow regions in the sense of first arrivals, such as an anomaly with large slowness $S(\mathbf{x})$ corresponding to stones or other blocks. It is, therefore, very challenging for using only first arrival signals for the inverse problem since the observed traveltimes at the boundary receivers are due to detoured rays which avoid these slow regions with large $S(\mathbf{x})$. In this paper, rather than providing an algorithm to improve the resolution, we propose to identify those regions in the reconstruction which is less reliable. As a result, this identification provides a reliability measure for the inversion.

Here we propose a labeling method to achieve this. The idea is to introduce a labeling function $F(\mathbf{x})$ such that it has a value 1 if \mathbf{x} is in the illuminated region and it equals 0 otherwise. Consider a ray arriving at a receiver \mathbf{x}^* on the boundary, parameterized by $\mathbf{x} = \mathbf{x}(s)$ where s is the arc-length parameter. We hope that $F(\mathbf{x}) \equiv 1$ along the ray $\mathbf{x} = \mathbf{x}(s)$, or equivalently

$$\frac{\mathrm{d}F(\mathbf{x}(s))}{\mathrm{d}s} = 0\tag{61}$$

which also implies

$$\nabla F(\mathbf{x}) \cdot \frac{\mathrm{d}\mathbf{x}(s)}{\mathrm{d}s} = 0.$$
(62)

Recalling the characteristics system of the eikonal equation [13], we have

$$\frac{\mathrm{d}\mathbf{x}(s)}{\mathrm{d}s} = \frac{\nabla T(\mathbf{x})}{S(\mathbf{x})}.\tag{63}$$

Plugging (63) into (62), we have

$$\nabla F(\mathbf{x}) \cdot \nabla T(\mathbf{x}) = 0. \tag{64}$$

Thus we get an advection equation for the required labeling function and $F(\mathbf{x})$ can be solved together with the boundary condition $F|_{\Gamma} = 1$, where Γ is the location of boundary receivers. However, to respect the flow direction of the characteristics, we propose to numerically solve

$$-\nabla F(\mathbf{x}) \cdot \nabla T(\mathbf{x}) = 0$$

$$F|_{\Gamma} = 1, \qquad (65)$$

so that the characteristics are inflow towards the point source.

In the joint transmission-reflection tomography there are two branches of signals: the transmission ray $T_t(\mathbf{x})$ and the reflection ray $T_r(\mathbf{x})$. Thus we introduce two labeling functions $F_t(\mathbf{x})$ and $F_r(\mathbf{x})$ to follow these rays respectively,

$$-\nabla F_t(\mathbf{x}) \cdot \nabla T_t(\mathbf{x}) = 0, \qquad \mathbf{x} \in \Omega$$

$$F_t(\mathbf{x}) = 1, \qquad \mathbf{x} \in \Gamma_2$$
(66)

and

$$-\nabla F_r(\mathbf{x}) \cdot \nabla T_r(\mathbf{x}) = 0, \qquad \mathbf{x} \in \Omega_1$$

$$F_r(\mathbf{x}) = 1, \qquad \mathbf{x} \in \Gamma_1.$$
(67)

And so the labeling function used to indicate the illuminated region in Ω is defined as

$$F(\mathbf{x}) = \max\left\{F_t(\mathbf{x}), F_r(\mathbf{x})\right\}.$$
(68)

The above derivation is for one data set corresponding to a single point source \mathbf{x}_s . For the multiple data sets as mentioned in section 3.4, we have multiple point sources $\{\mathbf{x}_s^j, j = 1, 2, \dots, N\}$ corresponding to multiple times of experiments. Then the labeling function $F(\mathbf{x})$ is defined as

$$F(\mathbf{x}) = \frac{1}{N} \sum_{j=1}^{N} F_j(\mathbf{x})$$
(69)

where each $F_j(\mathbf{x})$ is generated by equations (66-68) using transmission traveltime $T_t^j(\mathbf{x})$ and reflection traveltime $T_r^j(\mathbf{x})$ corresponding to the *j*-th point source \mathbf{x}_s^j . We can expect that in the region with a larger $F(\mathbf{x})$ (closer to 1) the slowness reconstruction $S(\mathbf{x})$ is more reliable.

5 Numerical implementation

In this section, we summarize the above algorithm and discuss the numerical implementation in details.

5.1 Algorithm for slowness reconstruction

- Step 1. Initialize ϕ^k , S_1^k and S_2^k for k = 0.
- Step 2. Construct $S(\mathbf{x})$ using (7).
- Step 3. Obtain $T_{t,j}(\mathbf{x})$ and $T_{r,j}(\mathbf{x})$ by solving (1-2) and (3-4) for each point source \mathbf{x}_s^j , $j = 1, 2, 3, \dots N$.
- Step 4. Obtain $\lambda_j(\mathbf{x})$, $\mu_j(\mathbf{x})$ and $\hat{\mu}_j(\mathbf{x})$ by solving the adjoint state equations (53-55) respectively, for $j = 1, 2, 3, \dots N$.
- Step 5. Compute $\tilde{\phi}^k$, \tilde{S}_1^k and \tilde{S}_2^k using the formula (58), (59) and (60), respectively.
- Step 6. Update $\phi^{k+1} = \phi^k + \epsilon \cdot \nu \tilde{\phi}^k$, $S_1^{k+1} = S_1^k + \epsilon \cdot \tilde{S}_1^k$, and $S_2^{k+1} = S_2^k + \epsilon \cdot \tilde{S}_2^k$.
- Step 7. Re-initialize ϕ^{k+1} by solving (39-40), and use Φ to update ϕ^{k+1} .
- Step 8. Go back to step 2 until the mismatch energy $E \leq \delta$ or the iteration step $k \geq k_{\max}$ for some given convergence parameters δ and k_{\max} .

Numerically, the Hamilton-Jacobi equation in step 3 can be efficiently solved using the fast sweeping methods [46, 22, 54, 35, 36]. In this work, we follow [54] and have implemented the local solver based on the Godunov Hamiltonian. For the reflection traveltime T_r the system of (3-4) is defined in $\Omega_1 \subset \Omega$, which is usually a non-square domain. To maintain a finite difference discretization we solve T_r in the whole domain Ω and impose the boundary condition using the level set function $\phi(\mathbf{x})$. Specifically, since $\phi(\mathbf{x})$ is maintained to be the signed distance to R, we have $\phi(\mathbf{x}) < 0$ in Ω_1 while $\phi(\mathbf{x}) > 0$ in Ω_2 ; consequently, the boundary condition (4) is implemented by setting

$$T_r(\mathbf{x}) = T_t(\mathbf{x}), \quad \mathbf{x} \in \{\mathbf{x} : \phi(\mathbf{x}) \ge 0\}$$
(70)

and we solve (3) in the whole domain Ω but only update $T_r(\mathbf{x})$ when $\phi(\mathbf{x}) < 0$.

In step 4, we solve the adjoint state equations (53-55); this is also achieved using the fast sweeping method and a detailed numerical discretization description can be found in [26, 28]. For example, to solve the advection equation

$$a \cdot \frac{\partial F}{\partial x} + b \cdot \frac{\partial F}{\partial y} = 0.$$

we have the following scheme:

$$\left[a_{i,j}^{+} \cdot \frac{F_{i,j} - F_{i-1,j}}{\Delta x} + a_{i,j}^{-} \cdot \frac{F_{i+1,j} - F_{i,j}}{\Delta x}\right] + \left[b_{i,j}^{+} \cdot \frac{F_{i,j} - F_{i,j-1}}{\Delta y} + b_{i,j}^{-} \cdot \frac{F_{i,j+1} - F_{i,j}}{\Delta y}\right] = 0, \quad (71)$$

where we denote $a^+ = \max\{a, 0\}$ and $a^- = \min\{a, 0\}$. (71) implies that

$$\left(\frac{a_{i,j}^{+} - a_{i,j}^{-}}{\Delta x} + \frac{b_{i,j}^{+} - b_{i,j}^{-}}{\Delta y}\right) \cdot F_{i,j} = \frac{a_{i,j}^{+} \cdot F_{i-1,j} - a_{i,j}^{-} \cdot F_{i+1,j}}{\Delta x} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j-1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j+1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j+1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j+1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j+1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j+1} - b_{i,j}^{-} \cdot F_{i,j+1}}{\Delta y} + \frac{b_{i,j}^{+} \cdot F_{i,j+1}}$$

and this gives an expression to build up a fast sweeping-type iterative method. A recent article [6] contains an analysis of this numerical approach. Here we mention the treatment of the boundary conditions for (54) and (55), which aims to maintain the finite difference discretization in the non-square domain Ω_1 .

Firstly, we study the location of the reflector R, which is the non-structured part of $\partial\Omega_1$. Mathematically the reflector R is expressed by $R = \phi^{-1}(0)$. Numerically however we may have no exactly zero-valued $\phi(\mathbf{x})$ at any grid point. To be consistent with the boundary treatment (70) for the solution of $T_r(\mathbf{x})$, we locate the numerical reflector R using the following strategy: a grid point $\mathbf{x}_{i,j}$ is labeled to be the numerical reflector if

$$0 \le \phi(\mathbf{x}_{i,j}) < \delta$$
 ($\delta = 3\Delta x$ in this implementation)

and

$$\{\phi(\mathbf{x}_{i-1,j}) < 0, \text{ or } \phi(\mathbf{x}_{i+1,j}) < 0, \text{ or } \phi(\mathbf{x}_{i,j-1}) < 0, \text{ or } \phi(\mathbf{x}_{i,j+1}) < 0\}$$
.

Then we study (54-55) in the whole domain Ω . For (54), we extend the coefficient $\nabla T_{r,j}$ to the whole Ω by setting

$$\nabla T_{r,j} = \begin{cases} \nabla T_{r,j} &, \quad \mathbf{x} \in \Omega_1 \cup R\\ 0 &, \quad \mathbf{x} \in \Omega \setminus (\Omega_1 \cup R) \end{cases}$$

where $\Omega_1 = {\mathbf{x} : \phi(\mathbf{x}) < 0}$ and R is the numerical reflector indicated as above. And the fast sweeping iteration is performed in the whole Ω with initial guess $\mu_j = 0$ everywhere. One finds that in the region $\nabla T_{r,j} = 0$, μ_j is not updated. Thus we actually compute μ_j in $\Omega_1 \cup R$ and extend the value to Ω automatically with $\mu_j = 0$ in $\Omega \setminus (\Omega_1 \cup R)$. The value of $\mu_j|_R$ is necessary because in (55) we need this boundary condition on R.

For (55), the coefficient $\nabla T_{t,i}$ is set to be

$$\nabla T_{t,j} = \begin{cases} \nabla T_{t,j} &, \mathbf{x} \in \Omega_1 \\ 0 &, \mathbf{x} \in \Omega \setminus \Omega_1 \end{cases}$$

and the fast sweeping iteration is performed in Ω with initial guess $\hat{\mu}_j = 0$ everywhere. Again one finds that we only update $\hat{\mu}_j$ in Ω_1 and extend the value to the whole Ω automatically with $\hat{\mu}_j = 0$ in $\Omega \setminus \Omega_1$. We mention that the gradient of the traveltime is calculated using the third order WENO scheme [29] in the inner grids while using first order upwind scheme near the boundary.

Lastly, we provide a local level set implementation in updating $\phi(\mathbf{x})$, which aims to reduce the computational complexity. Based on (7) for the slowness distribution, the level set function $\phi(\mathbf{x})$ mainly contributes near the reflector $R = \phi^{-1}(0)$. Thus we can update the value of ϕ only in a small tube containing R, and the re-initialization strategy maintains ϕ the signed distance function. Specifically, in steps 5 and step 6 we evaluate $\tilde{\phi}^k$ and update ϕ^{k+1} only in the computational tube $\{\mathbf{x} : |\phi(\mathbf{x})| < \epsilon_{\text{local}}\}$, where ϵ_{local} is a parameter controlling the width of the tube. This strategy helps to improve the computation since we do not need to determine $\tilde{\phi}(\mathbf{x})$ and $\phi^{\text{new}}(\mathbf{x})$ for all location in the whole computational domain.

5.2 Algorithm for identifying the illuminated region

- Step 1. Apply the reconstructed slowness $S(\mathbf{x})$ into (1-2) and equations (3-4) to solve $T_{t,j}(\mathbf{x})$ and $T_{r,j}(\mathbf{x})$ for each point source \mathbf{x}_{s}^{j} , $j = 1, 2, 3, \dots N$.
- Step 2. For $j = 1, 2, 3, \dots N$, obtain $F_{t,j}(\mathbf{x})$ and $F_{r,j}(\mathbf{x})$ by solving (66) and (67), and then generate $F_j(\mathbf{x}) = \max\{F_{t,j}(\mathbf{x}), F_{r,j}(\mathbf{x})\}.$
- Step 3. Obtain $F(\mathbf{x}) = \frac{1}{N} \sum_{j=1}^{N} F_j(\mathbf{x})$.



Figure 2: (Example 1) Initial guess of $S(\mathbf{x})$.

In step 2, we use also the fast sweeping method developed in [26, 28] to solve the advection equation. Note that to guarantee $F(\mathbf{x}) = 0$ in the unilluminated region, we initially set $F(\mathbf{x}) = 0$ everywhere before the sweeping. Also, we update $F_{i,j}$ only in the interior region of Ω , and set $F_{i,j} = 0$ on the boundary if there is no receivers. This is because eikonal solvers based on the fast sweeping approach usually generates artificial creeping ray along the boundary [15] and we do not want such artificial ray polluting the computation of our labeling function.

Furthermore, the advection system (67) is defined in $\Omega_1 \subset \Omega$ which is usually non-rectangular. To maintain a finite difference discretization, we extend (67) to the whole Ω by simply setting

$$\nabla T_r(\mathbf{x}) = \begin{cases} \nabla T_r(\mathbf{x}) &, \quad \mathbf{x} \in \Omega_1 \\ 0 &, \quad \mathbf{x} \in \Omega \setminus \Omega_1 \end{cases}$$

where $\Omega_1 = {\mathbf{x} : \phi(\mathbf{x}) < 0}, \ \Omega \setminus \Omega_1 = {\mathbf{x} : \phi(\mathbf{x}) \ge 0}$ and $\phi(\mathbf{x})$ is the level set function in the reconstructed $S(\mathbf{x})$. Then we perform the fast sweeping iteration for (67) in Ω but $F_r(\mathbf{x})$ is updated only in $\Omega_1 = {\mathbf{x} : \phi(\mathbf{x}) < 0}$.

6 Numerical examples

In this section, we test our algorithm on some numerical examples. In the first three examples, the computational domain is set to be $\Omega = [-1, 1] \times [0, 2]$ which is then discretized using 65×65 mesh grids. We assume N = 49 point sources located along one side of the domain: $(x_s^j, z_s^j) = (-0.96 + 0.04 \cdot (j-1), 0.05)$, $j = 1, 2, \dots, N$. In the last example, we consider a three dimensional example where the domain $\Omega = [-1, 1] \times [-1, 1] \times [0, 2]$ is discretized by a $65 \times 65 \times 65$ mesh. We put N = 49 point sources on one side of the domain: $(x_s^i, y_s^j, z_s) = (-0.9 + 0.3 \cdot (i-1), -0.9 + 0.3 \cdot (j-1), 0.05)$, $i, j = 1, 2, \dots, 7$. In all these examples, we have receivers on all the grid nodes along $\Gamma_2 = \{z = 2\}$ to record the transmission traveltime T_t , and we put receivers on all the grid nodes along $\Gamma_1 = \{z = 0\}$ to record the reflection traveltime T_r .

In all following examples, the smoothing parameter τ in the numerical Heaviside function $H_{\tau}(\mathbf{x})$ is chosen to be $\tau = 0.01$, and the updating step size is fixed to be $\epsilon = 10^{-3}$. The parameter to reduce the perturbation of ϕ is $\nu = 0.1$, the weight of the regularization term in ϕ is $\gamma = 0.01$, and the weight in controlling the amount of regularity in \tilde{S}_1 and \tilde{S}_2 is $\alpha = 1$. Furthermore, the width of the computational tube for the local level set implementation is set to be $\epsilon_{\text{local}} = 4\Delta x$. The initial guess for the level set function $\phi(\mathbf{x})$ is always set to be the signed distance to z = 1, i.e. $\phi^0(\mathbf{x}) = z - 1$.

6.1 Example 1

In this example the reflector is located at $z = 2 - \sqrt{1.5^2 - x^2}$ and the slowness distribution is

$$S(x,z) = \begin{cases} S_1(x,z) &, z \le 2 - \sqrt{1.5^2 - x^2} \\ S_2(x,z) &, z > 2 - \sqrt{1.5^2 - x^2} \end{cases}$$



Figure 3: (Example 1, case 1) Piecewise homogeneous structure.



Figure 4: (Example 1, case 2) Piecewise continuous structure.



Figure 5: (Example 2) Initial guess of $S(\mathbf{x})$.



Figure 6: (Example 2, case 1) Piecewise homogeneous structure.



Figure 7: (Example 2, case 2) Piecewise continuous structure.



Figure 8: (Example 3, case 1) Piecewise homogeneous structure.



Figure 9: (Example 3, case 2) Piecewise continuous structure.



Figure 10: (Example 4, case 1) 3D tomography, piecewise homogeneous structure. (a)-(c) and (g)-(i): Exact slowness with slices x = -1, 0, 1 and y = -0.5, 0, 0.5. (d)-(f) and (j)-(l): Results after 2000 iterations with slices x = -1, 0, 1 and y = -0.5, 0, 0.5.



Figure 11: (Example 4, case 2) 3D tomography, piecewise continuous structure. (a)-(c) and (g)-(i): Exact slowness with slices x = -1, 0, 1 and y = -0.5, 0, 0.5. (d)-(f) and (j)-(l): Results after 2000 iterations with slices x = -1, 0, 1 and y = -0.5, 0, 0.5.

We have tested two cases. In the first case, the medium is piecewise homogeneous with $S_1(x, z) = 1$ and $S_2(x, z) = 0.5$. We start the iteration with initial guess $S_1^0 = 1.5$, $S_2^0 = 0.3$ and $\phi^0(\mathbf{x}) = z - 1$. The initial slowness function $S(\mathbf{x})$ is shown in figure 2. Figure 3 provides the numerical results after 10000 iterations. One finds that the structure is well recovered and the error mainly appears in the region near the discontinuity. Also the illumination is clearly identified by our labeling function $F(\mathbf{x})$ in (d).

In the second case we test a piecewise continuous structure with

$$S_1(x,z) = 1 + 0.5 \cdot \exp(-16(x^2 + (z - 0.25)^2))$$

and $S_2(x, z) = 0.5$. The initial guess of $S(\mathbf{x})$ is the same as in case 1, as shown in figure 2. This test case is more challenging due to the heterogeneity. We perform 30000 iterations and figure 4 shows the numerical results. One finds that the shape of reflector is well recovered and the slowness distribution including the anomaly structure is well visualized.

6.2 Example 2

In this example, the reflector is located at $z = \sqrt{1.5^2 - x^2}$ and the slowness distribution is

$$S(x,z) = \begin{cases} S_1(x,z) &, z \le \sqrt{1.5^2 - x^2} \\ S_2(x,z) &, z > \sqrt{1.5^2 - x^2} \end{cases}$$

We have also tested two cases. In the first case, the medium is piecewise homogeneous with $S_1(x, z) = 1$ and $S_2(x, z) = 0.5$. We start the iteration with the initial guess $S_1^0 = 0.7$, $S_2^0 = 0.3$ and $\phi^0(\mathbf{x}) = z - 1$. The initial slowness function $S(\mathbf{x})$ is shown in figure 5. Figure 6 provides the numerical results after 10000 iterations. The piecewise structure is well obtained with a very good reconstruction of the reflector.

In the second case, we study a piecewise continuous structure with $S_1(x, z) = 1 + 0.3 \cdot \exp(-(x^2 + (z - 0.7)^2))$ and $S_2(x, z) = 0.5$. The initial guess of $S(\mathbf{x})$ is the same as in case 1, as shown in figure 5. Figure 7 shows the numerical results after 13000 iterations. From the plot of error (figure 7 (c)) one finds that the location of the reflector is perfectly recovered. Also we get a good inversion of the slowness distribution including the non-homogeneous structure beyond the reflector.

6.3 Example 3

In the third example, we test a sinusoidal reflector located at $z = 0.65 + 0.25 \sin(\pi x)$ and the slowness distribution is

$$S(x,z) = \begin{cases} S_1(x,z) &, z \le 0.65 + 0.25\sin(\pi x) \\ S_2(x,z) &, z > 0.65 + 0.25\sin(\pi x) \end{cases}$$

This is a relatively difficult example where the shape of reflector is more involved.

Still we have tested two cases, one with piecewise homogeneous structure and the other with heterogeneous structure. In both cases the initial guess for $S(\mathbf{x})$ is the same as that in example 1, as shown in figure 2. In the first case, we set $S_1(x, z) = 1$ and $S_2(x, z) = 0.5$. We perform 20000 iterations and the final numerical results are shown in figure 8. We get a perfect reconstruction for the shape of the reflector. In the recovered $S(\mathbf{x})$ as shown in (b), although there are shadow regions which deviate from the homogeneity, the basic structure is correct and the error is acceptable.

In the second case, the medium is piecewise continuous with

$$S_1(x,z) = 1 + 0.5 \cdot \exp\left(-\left(\frac{(x-0.5)^2}{0.2^2} + \frac{(z-0.4)^2}{0.4^2}\right)\right)$$

and $S_2(x, z) = 0.5$. We perform the iterations 11000 times and the numerical results are shown in figure 9. The shape of the reflector is well recovered. The anomaly in $S(\mathbf{x})$ is not perfect due to the difficult heterogeneity. However, the reconstruction in (b) still provides us very useful information to understand the structure.

6.4 Example 4

In the last example, we compute the three dimensional tomography inversion, where the reflector is located at $z = \sqrt{3.5^2 - x^2 - y^2} - 2$ with the slowness distribution is

$$S(x,y,z) = \begin{cases} S_1(x,y,z) &, z \le \sqrt{3.5^2 - x^2 - y^2} - 2\\ S_2(x,y,z) &, z > \sqrt{3.5^2 - x^2 - y^2} - 2 \end{cases}$$

Also we have tested two cases, for both tests we start iterations with the same initial guess given by $S_1^0(x, y, z) = 0.7$, $S_2^0(x, y, z) = 0.3$ and $\phi^0(x, y, z) = z - 1$.

In the first case, the medium is piecewise homogeneous with $S_1(x, y, z) = 1$ and $S_2(x, y, z) = 0.5$. Figure 10 shows the numerical results after 2000 iterations, where the 3D structure is presented by slices. We plot the slices of $S(\mathbf{x})$ at x = -1, 0, 1 and y = -0.5, 0, 0.5. The shape of the reflector is perfectly recovered and the deviation in the reconstructed slowness structure is acceptable. In the second case, the medium is heterogeneous with $S_1(x, z) = 1 + 0.3 \cdot \exp\left(-\left(x^2 + y^2 + (z - 0.7)^2\right)\right)$ and $S_2(x, z) = 0.5$. Figure 11 shows the numerical results after 2000 iterations. Solutions from both cases are obtained by a laptop PC with CPU speed 2.66GHz. The first example is solved in approximately 21 hours, while the second example takes about 24 hours.

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A Derivation of (15) and (16)

Consider the eikonal equation (1) which is valid for both $T_t(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2)$ and $T_t(\phi, S_1, S_2)$,

$$\left(\nabla T_t(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2)\right)^2 = S^2(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2), \tag{72}$$

$$(\nabla T_t(\phi, S_1, S_2))^2 = S^2(\phi, S_1, S_2).$$
(73)

Plugging formula (13) into (72) and subtracting (73) from (72), we get

$$2\epsilon\nabla T_t \cdot \nabla \tilde{T}_t + O(\epsilon^2) = S^2(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) - S^2(\phi, S_1, S_2).$$
(74)

From (8) and (9), we have

$$S(\phi + \epsilon \cdot \nu \tilde{\phi}, S_1 + \epsilon \tilde{S}_1, S_2 + \epsilon \tilde{S}_2) = S(\phi, S_1, S_2) + \epsilon \cdot \nu \tilde{\phi} \cdot \frac{S_2 - S_1}{2\tau \cdot \cosh^2 \frac{\phi}{\tau}} + \epsilon \tilde{S}_1 \cdot (1 - H_\tau(\phi)) + \epsilon \tilde{S}_2 \cdot H_\tau(\phi) + O(\epsilon^2).$$
(75)

Now, substituting (75) into (74), we obtain

$$2\epsilon\nabla T_t \cdot \nabla \tilde{T}_t + O(\epsilon^2) = 2\epsilon \cdot S(\phi, S_1, S_2) \cdot \left[\nu\tilde{\phi} \cdot \frac{S_2 - S_1}{2\tau \cdot \cosh^2 \frac{\phi}{\tau}} + \tilde{S}_1 \cdot (1 - H_\tau(\phi)) + \tilde{S}_2 \cdot H_\tau(\phi)\right] + O(\epsilon^2).$$
(76)

To simplify the notation, we denote

$$\begin{aligned} A(\phi, S_1, S_2) &= S(\phi, S_1, S_2) \cdot \frac{S_2 - S_1}{2\tau \cdot \cosh^2 \frac{\phi}{\tau}}, \\ B(\phi, S_1, S_2) &= S(\phi, S_1, S_2) \cdot (1 - H_\tau(\phi)), \\ C(\phi, S_1, S_2) &= S(\phi, S_1, S_2) \cdot H_\tau(\phi). \end{aligned}$$

Then, matching $O(\epsilon)$ terms in (76), we obtain

$$\nu \tilde{\phi} \cdot A(\phi, S_1, S_2) + \tilde{S}_1 \cdot B(\phi, S_1, S_2) + \tilde{S}_2 \cdot C(\phi, S_1, S_2) - \nabla T_t \cdot \nabla \tilde{T}_t = 0$$

which is (15).

Performing a similar calculation for T_r in the domain Ω_1 , we have the relation between $\tilde{\phi}$, \tilde{S}_1 , \tilde{S}_2 and \tilde{T}_r ,

$$\nu \dot{\phi} \cdot A(\phi, S_1, S_2) + \dot{S}_1 \cdot B(\phi, S_1, S_2) + \dot{S}_2 \cdot C(\phi, S_1, S_2) - \nabla T_r \cdot \nabla \dot{T}_r = 0,$$

which gives (16).

B Derivation of Lemma 3.1 and Lemma 3.2

B.1 Derivation of Lemma 3.1

Multiplying (15) by λ , integrating it over Ω and adding to (20), we get

$$\frac{\delta E}{\epsilon} = \int_{\Gamma_1} \tilde{T}_r (T_r - T_r^*) ds + \int_{\Gamma_2} \tilde{T}_t (T_t - T_t^*) ds + \int_{\Omega} \lambda (W - \nabla T_t \cdot \nabla \tilde{T}_t) d\mathbf{x} + O(\epsilon)$$

$$= \int_{\Gamma_1} \tilde{T}_r (T_r - T_r^*) ds + \int_{\Gamma_2} \tilde{T}_t (T_t - T_t^*) ds + \int_{\Omega} \lambda W d\mathbf{x}$$

$$+ \int_{\Omega} \operatorname{div}(\lambda \nabla T_t) \cdot \tilde{T}_t d\mathbf{x} - \int_{\partial \Omega} \lambda \frac{\partial T_t}{\partial \mathbf{n}} \cdot \tilde{T}_t ds + O(\epsilon),$$
(77)

where W is the abbreviation in formula (21) and **n** denotes the unit outward normal of $\partial\Omega$. From (77), we conclude that if λ satisfies the adjoint state equation (22),(23) and (24) given in Lemma 3.1, the perturbation of the mismatch energy reduces to

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W \mathrm{d}\mathbf{x} + \int_{\Gamma_1} \tilde{T}_r (T_r - T_r^*) \mathrm{d}s + O(\epsilon),$$

which is (25) in Lemma 3.1.

B.2 Derivation of Lemma 3.2

We want to eliminate the term \tilde{T}_r in δE by considering (16). With the abbreviation (21), we have

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W d\mathbf{x} + \int_{\Gamma_{1}} \tilde{T}_{r} (T_{r} - T_{r}^{*}) ds + \int_{\Omega_{1}} \mu (W - \nabla T_{r} \cdot \nabla \tilde{T}_{r}) d\mathbf{x} + O(\epsilon)$$

$$= \int_{\Omega} \lambda W d\mathbf{x} + \int_{\Gamma_{1}} \tilde{T}_{r} (T_{r} - T_{r}^{*}) ds + \int_{\Omega_{1}} \mu W d\mathbf{x}$$

$$+ \int_{\Omega_{1}} \operatorname{div}(\mu \nabla T_{r}) \cdot \tilde{T}_{r} d\mathbf{x} - \int_{\partial \Omega_{1}} \mu \frac{\partial T_{r}}{\partial \mathbf{n}} \cdot \tilde{T}_{r} ds + O(\epsilon).$$
(78)

At first glance, a natural consideration is to introduce μ which satisfies the following adjoint state equation

$$-\operatorname{div}(\mu\nabla T_r) = 0, \quad \text{in } \Omega_1 \tag{79}$$

$$\iota \frac{\partial T_r}{\partial \mathbf{n}} = T_r - T_r^*, \quad \text{on } \Gamma_1 \tag{80}$$

$$\mu = 0, \qquad \text{on } \partial\Omega_1 \setminus \Gamma_1, \tag{81}$$

and so \tilde{T}_r in (78) can be removed. However, studying (79) carefully, we find that the boundary condition (81) is not appropriate. In particular, we rewrite (79) in the following form

$$\nabla \mu \cdot (-\nabla T_r) + \mu (-\Delta T_r) = 0.$$
(82)

The characteristic of (82) is $\frac{d\mathbf{x}}{ds} = -\nabla T_r$ which leads to the following ODE system

$$\frac{\mathrm{d}\mu}{\mathrm{d}s} + \mu(-\Delta T_r) = 0.$$
(83)

Therefore the appropriate boundary condition requires $(-\nabla T_r) \cdot \mathbf{n} = -\frac{\partial T_r}{\partial \mathbf{n}} \leq 0$ such that along the characteristics the boundary information propagates inside the domain Ω_1 . While on the reflector $R \subset \partial \Omega_1 \setminus \Gamma_1$, one finds $-\frac{\partial T_r}{\partial \mathbf{n}} > 0$ which means the information of μ propagates from the inside region of Ω_1 to the reflector R and we cannot explicitly impose $\mu = 0$ on $R \subset \partial \Omega_1 \setminus \Gamma_1$.

To fix this problem, firstly we consider the adjoint state equation (26-28) given in Lemma 3.2,

$$\begin{aligned} -\operatorname{div}(\mu\nabla T_r) &= 0, & \text{in } \Omega_1 \\ \mu \frac{\partial T_r}{\partial \mathbf{n}} &= T_r - T_r^*, & \text{on } \Gamma_1 \\ \mu &= 0, & \text{on } \partial \Omega_1 \setminus (R \cup \Gamma_1), \end{aligned}$$

and so (78) reduces to

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W \mathrm{d}\mathbf{x} + \int_{\Omega_1} \mu W \mathrm{d}\mathbf{x} - \int_R \mu \frac{\partial T_r}{\partial \mathbf{n}} \cdot \tilde{T}_r \,\mathrm{d}s + O(\epsilon). \tag{84}$$

To eliminate \tilde{T}_r on R, we realize an important relation between T_t and T_r by (4). Since $T_r(\mathbf{x}) = T_t(\mathbf{x})$ on R, we have

$$\hat{T}_r(\mathbf{x}) = \hat{T}_t(\mathbf{x}), \quad \mathbf{x} \text{ on } R.$$
 (85)

Substituting (85) into (84), we get

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W \mathrm{d}\mathbf{x} + \int_{\Omega_1} \mu W \mathrm{d}\mathbf{x} - \int_R \mu \frac{\partial T_r}{\partial \mathbf{n}} \cdot \tilde{T}_t \,\mathrm{d}s + O(\epsilon).$$
(86)

One finds that the relation (15) can be utilized again to reduce the integrating term involving \tilde{T}_t . Multiplying (15) by $\hat{\mu}$, integrating it over Ω_1 and adding to (86), we have

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W d\mathbf{x} + \int_{\Omega_{1}} \mu W d\mathbf{x} - \int_{R} \mu \frac{\partial T_{r}}{\partial \mathbf{n}} \cdot \tilde{T}_{t} ds + \int_{\Omega_{1}} \hat{\mu} (W - \nabla T_{t} \cdot \nabla \tilde{T}_{t}) d\mathbf{x} + O(\epsilon)$$

$$= \int_{\Omega} \lambda W d\mathbf{x} + \int_{\Omega_{1}} \mu W d\mathbf{x} - \int_{R} \mu \frac{\partial T_{r}}{\partial \mathbf{n}} \cdot \tilde{T}_{t} ds$$

$$+ \int_{\Omega_{1}} \hat{\mu} W d\mathbf{x} + \int_{\Omega_{1}} \operatorname{div}(\hat{\mu} \nabla T_{t}) \cdot \tilde{T}_{t} d\mathbf{x} - \int_{\partial\Omega_{1}} \hat{\mu} \frac{\partial T_{t}}{\partial \mathbf{n}} \cdot \tilde{T}_{t} ds + O(\epsilon).$$
(87)

Then the adjoint state equation for $\hat{\mu}$ is

$$-\operatorname{div}(\hat{\mu}\nabla T_t) = 0, \quad \text{in } \Omega_1 \tag{88}$$

$$\hat{\mu}\frac{\partial I_t}{\partial \mathbf{n}} = -\mu\frac{\partial I_r}{\partial \mathbf{n}}, \qquad \text{on } R \tag{89}$$

$$\hat{\mu} = 0, \quad \text{on } \partial\Omega_1 \setminus R,$$
(90)



Figure 12: Notation used in simplifying the boundary condition (89).

where (88) is (29) and (90) is (31) in Lemma 3.2. And so the mismatch energy finally reduces to (32),

$$\frac{\delta E}{\epsilon} = \int_{\Omega} \lambda W \mathrm{d}\mathbf{x} + \int_{\Omega_1} (\mu + \hat{\mu}) W \mathrm{d}\mathbf{x} + O(\epsilon) \,.$$

We can further simplify the boundary condition (89) in the adjoint state equation for $\hat{\mu}$. As shown in Figure 12, we have $|\nabla T_t(\mathbf{x})| = |\nabla T_r(\mathbf{x})| = S(\mathbf{x})$ at the point $\mathbf{x} \in R$ due to the eikonal equation. And so

$$\frac{\partial T_t}{\partial \mathbf{n}} = \nabla T_t \cdot \mathbf{n} = |\nabla T_t| \cdot |\mathbf{n}| \cdot \cos \theta = S(\mathbf{x}) \cdot \cos \theta$$
$$\frac{\partial T_r}{\partial \mathbf{n}} = \nabla T_r \cdot \mathbf{n} = |\nabla T_r| \cdot |\mathbf{n}| \cdot \cos(\pi - \theta) = -S(\mathbf{x}) \cdot \cos \theta,$$

which imply that

$$\frac{\partial T_t}{\partial \mathbf{n}} = -\frac{\partial T_r}{\partial \mathbf{n}}.\tag{91}$$

Plugging (91) into (89), we finally obtain the simplified boundary condition (30) given by

$$\hat{\mu} = \mu$$
, on R .