Source estimation for Wave Equations with uncertain parameters

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Abstract—Source estimation is a fundamental ingredient of Full Waveform Inversion (FWI). In such seismic inversion methods waveform intensity and phase spectra are usually estimated statistically although for the FWI formulation as a nonlinear least-squares optimization problem it can naturally be incorporated to the workflow. Modern approaches for source estimation consider robust misfit functions leading to the well known robust FWI method. The present work uses synthetic data generated from a high order spectral element forward solver to produce observed data which in turn are used to estimate the intensity and the location of the point seismic source term of the original elastic wave PDE. A min-max filter approach is used to convert the original source estimation problem into a state problem conditioned to the observations and a non-standard uncertainty description. The resulting numerical scheme uses an implicit midpoint method to solve, in parallel, the chosen 2D and 3D numerical examples running on an IBM Blue Gene/Q using a grid defined by approximately sixteen thousand $5^{th}$ order elements, resulting in a total of approximately 6.5 million degrees of freedom.

I. INTRODUCTION

Source estimation is an essential ingredient of the Full Waveform Inversion (FWI) technique since the inferred shape and location of the seismic wavelet may strongly influence the seismic inversion results and the subsequent assessments of the quality of the reservoir model. In seismic inversion methods like FWI, wavelet intensity/amplitude and phase spectra are usually estimated statistically from seismic data alone or from a combination of seismic data and available well measurements such as sonic and density curves. After the seismic wavelet is estimated, it is used to compute seismic reflection coefficients in the inversion process. A reliable wavelet estimate allows for better trace inversion, spike deconvolution, line-mistrying correction as well as forward modeling [7]. In the context of FWI formulation as a nonlinear least-squares optimization problem, source estimation can naturally be incorporated by choosing the source weights for a given model to be a minimizer of a least-squares misfit function [8]. Most recent approaches for source estimation consider variable projection for nonlinear least-squares [4] and robust misfit using twice differentiable misfit functions [1], [9].

In this work, synthetic data generated by a high order spectral element forward solver produce observed data which are used to estimate the intensity and the location of the point seismic source term of the original elastic wave PDE. The elastic wave equation in displacement formulation is discretized by using the spectral element method and an Ordinary Differential Equation (ODE) is derived to approximate the dynamics of the projection coefficients. The latter are, in fact, approximations of the values of the displacement filed over the set of grid points. It is then assumed that the source term is absolutely continuous function of time with unknown but bounded derivative. We also assume that at initial time the source intensity equals zero. The latter assumptions allow us to introduce an additional differential equation for the source term. A min-max filter approach [2], [6], [5] is then applied to this extended ODE in order to derive the estimate of the artificial state representing the source term. The equations for the filter and the minimax gain are then discretized by using an implicit mid-point method which preserves quadratic invariants. The numerical experiments conducted for smooth (Ricker wavelet) and non-smooth (rectangular function) sources, and 2D and 3D wave equations prove the efficacy of our approach.

II. NOTATION

Let $\Omega \subset \mathbb{R}^3$ denote a computational solid domain with boundary $\Gamma$ and set $\Omega_T := \Omega \times [t_{\min}, t_{\max}]$. $L^2(\Omega_T)$ denotes the space of square integrable functions over $\Omega_T$. In what follows we employ Einstein summation notation, that is summation is implied over the repeated index. For instance, $\partial_{x_i} \sigma_{ij} = \sum_j \partial_{x_j} \sigma_{i,j}$ where $\sigma_{ij}(x)$ is a component of stress tensor field $\sigma$.

III. PROBLEM STATEMENT

The elastic wave equation is a statement of Newton’s second law of motion applied to a continuous solid material and is defined in $\Omega_T$ as:

$$\rho \partial_t u_i = \partial_{x_i} \sigma_{ij} + f_i$$

where $i, j \in [1-3], t \in [t_{\min}, t_{\max}], x \in \Omega, u_i(x, t)$ is the $i$-th component of the displacement vector field, $\rho(x)$ is the density, $f_i(x, t)$ is the seismic source, modeled in the form of a point source:

$$f_i(x, t) = \theta(t) \delta(x_i - x_i, \text{source})$$

and $\sigma_{ij}$ is the stress tensor field, modeled with the linear constitutive relation

$$\sigma_{ij} = c_{ijkl} \varepsilon_{kl} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij}$$
where \( c_{ijkl} \) denotes a general \( 4^{th} \) order elasticity tensor and \( \varepsilon_{ij} \) the strain tensor, and specifically for a linear elastic solid, \( \lambda(x) \) and \( \mu(x) \) are the first and second Lamé parameters respectively. The elastic wave equation is subject to the standard initial conditions \( u_i = \partial_t u_i = 0 \), free surface boundary conditions

\[
\sigma_{ij} n_j = 0,
\]

and Clayton and Enquist absorbing boundary conditions

\[
\sigma_{ij} n_j = -\rho v \partial_t u_i
\]

respectively, where \( n_j \) denotes the normal to the boundary \( \Gamma \) and \( v \) denotes the elastic wave speed (which will be \( P \) wave speed for displacement components parallel to \( n_j \) and \( S \) wave speed for components perpendicular to \( n_j \)).

Assume that a function \( Y \) is observed in the form:

\[
Y(x, y, z, t) = \int_{\Omega_T} g(x - x', y - y', z - z', t - t') \times u(x', y', z', t') dx'dy'dz'dt' + \eta(x, y, t),
\]

where \( g \in L^2(\Omega_T) \) is an averaging kernel and \( \eta \) models an observation noise. Given the data \( Y \), we would like to estimate the position \( x_{i, \text{source}} \) and intensity \( \theta \) of the source term \( f \).

### IV. REVIEW OF THE SPECTRAL ELEMENT METHOD FOR ELASTIC WAVE EQUATION

Using the Spectral Element Method, the computational domain is defined as a tessellation of hexahedral elements with the displacement field approximated as \( u_i(x, t) \approx u_{i,pqr}(t) \psi_{pqr}(x) \), which combined with Galerkin projection gives the weak form:

\[
\int_{\Omega^e} \psi_{abc} \rho \psi_{pqr} \partial_t u_{i,pqr} d\Omega + \int_{\Gamma^e} \psi_{abc} \rho v \psi_{pq} \partial_t u_{i,pq} d\Gamma + \int_{\Omega^e} \partial_{x_j} \psi_{abc} c_{ijkl} \frac{1}{2} \left( \partial_{x_i} \psi_{pqr} u_{k,pqr} + \partial_{x_k} \psi_{pqr} u_{i,pqr} \right) d\Omega = \int_{\Omega^e} \psi_{abc} f_i d\Omega.
\]

In this specific implementation the basis functions \( \psi_{pqr} \) are taken to be a tensor product of the family of \( N^{th} \) order Lagrange polynomials \( \psi_{pqr} = \ell_p \ell_q \ell_r \), which integrating over a reference element with Gauss-Legendre-Lobatto (GLL) quadrature, gives the elemental matrices:

\[
M_{i,j,abc,pqr}^{(e)} = \sum_{f,g,h=1}^{N+1} w_f w_g w_h \psi_{abc} \partial_{y_q} \psi_{pqr} J |_{\xi_1,f,\xi_2,g,\xi_3,h}^e
\]

\[
K_{i,j,abc,pqr}^{(e)} = \sum_{f,g,h=1}^{N+1} w_f w_g w_h \partial_{\xi_k} \psi_{abc} \left( \frac{\partial \xi_k}{\partial x_l} \right) \frac{1}{2} c_{ijkl} J |_{\xi_1,f,\xi_2,g,\xi_3,h}^e
\]

\[
C_{i,j,abc,pq}^{(e)} = \sum_{f,g,h=1}^{N+1} w_f w_g w_h \partial_{\xi_m} \psi_{abc} \psi_{pq} J |_{\xi_1,f,\xi_2,g}^e
\]

where \( \xi_i \in [-1, +1] \) denote the coordinates of the reference element, \( J \) defines the Jacobian of the transformation mapping a given element to the reference, and \( w_i \) denote the weights associated with the GLL quadrature. The elemental matrices may be assembled into their global counterparts, defining the system of ODEs

\[
M\ddot{u} + C\dot{u} + K u = s
\]

where \( M, C, K \), and \( s \) are the global mass, damping, stiffness matrices, and source vector. Initial conditions are given as follows: \( s(t_{\text{min}}) = s(t_{\text{max}}) = 0 \). We stress that \( u \) models projection coefficients representing the solution of the wave equation (1) in the basis of the finite dimensional space spanned by the Lagrange polynomials \( \psi_{pqr} = \ell_p \ell_q \ell_r \).

In fact, \( u \) “lives” in the physical space and represents the approximation of the values of the displacement field \( u_i \) over the set of chosen GLL quadrature points.

It was recognized in [11], [12] that the approximation error of the spectral element method, as well as any Galerkin projection method, may be modelled as an uncertain but bounded input \( g \) in the following form:

\[
M\ddot{u} + C\dot{u} + K u = s + g
\]

Accounting for the projection error allows one to increase the approximation quality of the model (5).

Now, in order to relate the observed data \( Y(x, y, z, t) \) to the projection coefficients \( u \) described by (6) we also project the observation equation (2) onto the span of the Lagrange polynomials. As a result we arrive at the following system:

\[
Y(t) = H u + e(t),
\]

where \( e(t) \) denotes the observation error and the matrix \( H \) describes the locations of the receivers in \( \Omega \). We further assume that \( e(t) \) is a realisation of a random process with zero mean and a given covariance function \( R(t) \).

Now, we would like to estimate the position and intensity of the source term \( s \) assuming that

\[
s = Bf
\]

and \( f = g(t) \) where \( B \) is a matrix representing a possible spatial localisation of the source term. We stress that, in general, we do not require any knowledge about source.
Also we note that $R$ values of the error in the observations (roughly speaking: high eigen and uncertainty description belongs to this ellipsoid. As a solution” of (9) which is compatible with the observed data and together with the projection error term satisfies the following inequality:

$$\int_{t_{\text{min}}}^{t_{\text{max}}} \|g(t)\|^2 + \|\mathbf{g}\|^2 dt \leq \mu^2,$$

(8)

where $\mu$ is a given scalar.

V. MIN-MAX SOURCE ESTIMATOR

Now, let us describe the estimation procedure. To this end, we extend (6) with an additional equation:

$$M \ddot{\mathbf{u}} = B \dot{\mathbf{f}} + \mathbf{g} - C \dot{\mathbf{u}} - K \mathbf{u}, \quad \mathbf{u}(0) = \ddot{\mathbf{u}} = 0, \quad \mathbf{f}(0) = 0. \quad (9)$$

so that the source estimation problem now becomes a state estimation problem: estimate $B \dot{\mathbf{f}}(t^*)$, taking into account observations, $Y(t)$, and a non-standard uncertainty description (random noise in observations and deterministic projection error together with uncertain but bounded-in-energy time derivative of the source term in the state equation (9)). We stress that each component of $s$ represents the value of the continuous source term $f$ at a certain GLL point and so we simultaneously estimate position and intensity of $f$ over the grid imposed on $\Omega$.

Taking into account the aforementioned uncertainty description (ellipsoid (8)), a minimax state estimation [2], [6], [5] is a natural choice in order to construct a robust estimate of $f(t^*)$. Assume that $t^*$ is $t_{\text{max}}$. We construct a minimax filter to estimate $f(t^*)$. Namely, we define an extended state vector $\mathbf{x}(t) = (\mathbf{u}, \dot{\mathbf{u}}, \mathbf{f}(t))^T$, extended state transition and observation matrices

$$A := \begin{pmatrix} 0 & 0 & 1 \\ -M^{-1}K & -M^{-1}C & M^{-1}B \end{pmatrix}, \quad H_e = \begin{pmatrix} H & 0 & 0 \end{pmatrix}$$

Then (9) is equivalent to the following system of ODEs:

$$\dot{\mathbf{x}} = A \mathbf{x} + W \mathbf{g},$$

where $W = [0, I]$. Now, we remind that $R$ corresponds to the error in the observations (roughly speaking: high eigen values of $R$ correspond to low error and on the contrary). Also we note that $\mu$ defines the energy of the model error $g$: big $\mu$ corresponds to large model error $g$.

Following [10] we introduce the following equations for the estimator $\hat{\dot{\mathbf{x}}}$:

$$\dot{\mathbf{x}} = A \mathbf{x} + \hat{P}(t)H_e Y(t) - H_e \ddot{\mathbf{x}}, \quad \mathbf{x}(t_{\text{min}}) = \hat{\mathbf{x}}(t_{\text{min}}) = 0,$$

$$\hat{P} = AP + PA^T + \mu WW^T - PH_e H_e^T \hat{P}, \quad \hat{P}(t_{\text{min}}) = 0. \quad (10)$$

Note that $P$ is an analogue of the state error covariance matrix of the Kalman Filter, and for each time instant $t$ it defines an ellipsoid centered around $\hat{\dot{\mathbf{x}}}(t)$ so that any “true solution” of (9) which is compatible with the observed data and uncertainty description belongs to this ellipsoid. As a result we obtain a guaranteed estimate of the state vector $\mathbf{x}(t) = (\mathbf{u}, \dot{\mathbf{u}}, s(t))^T$.

If $t^* = t_{\text{min}}$, then one needs to apply a variational method to estimate $\mathbf{x}(t^*)$. Namely, we need to solve the 2-point boundary value problem:

$$\dot{\mathbf{x}} = A\dot{\mathbf{x}} + PH_e R(Y(t) - H_e \dot{\mathbf{x}}), \quad \mathbf{z}(t_{\text{max}}) = 0,$$

$$\mathbf{z} = -A^T \mathbf{z} - H_e R(Y(t) - H_e \dot{\mathbf{x}}), \quad \mathbf{z}(t^*) = \hat{\mathbf{x}}(t^*). \quad (11)$$

If $t_{\text{min}} < t^* < t_{\text{max}}$ then one may first apply filtering to get the estimate of $\mathbf{x}(t^*)$ and then improve the obtained estimate $\mathbf{x}(t^*)$ by using it in (11). This allows us to take into account the entire dataset and leads, in general, to improved estimates of $s(t^*)$.

In what follows we concentrate on the case $t^* = t_{\text{max}}$ for simplicity.

VI. STRUCTURE PRESERVING TIME INTEGRATION FOR THE MIN-MAX ESTIMATOR

In order to construct a numerical approximation for (10), we note that (9) is stiff and so implicit methods are preferable. In addition, the eigenvalues of $P(t)$ define the size of the ellipsoid containing $\ddot{\mathbf{x}}(t)$ and so to get reliable error estimates, the chosen numerical method should preserve quadratic invariants (for instance, the Frobenius norm of $P(t)$). We recall that the solution $P$ of the Riccati equation may be derived from Hamiltonian system:

$$\begin{pmatrix} dU/dt \\ dV/dt \end{pmatrix} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \begin{bmatrix} -\mu W W^T & A^T \\ H_e^T R H_e & A \end{bmatrix} \begin{pmatrix} U \\ V \end{pmatrix}. \quad (12)$$

Indeed, by straightforward differentiation it is easy to check that $P = VU^{-1}$. By noting that the latter equation for $U$ and $V$ is Hamiltonian, we apply implicit midpoint method in order to construct numerical approximations for $U$, $V$ and $P$. Namely, we define: $P_n = V_n U_n^{-1}$ for $n > 0$ and $P_0 = 0$ and set $P_{in} = V_{in} U_{in}^{-1}$ where $U_n$, $V_n$ and $U_{in}$, $V_{in}$ are defined from the following equations:

$$U_{n+1} = U_n + h \sum_{i=1}^{2} \delta U_{in} ,$$

$$V_{n+1} = V_n + h \sum_{i=1}^{2} \delta V_{in} ,$$

$$V_{in} = V_n + h \sum_{j=1}^{2} \delta V_{jn} ,$$

$$U_{in} = U_n + h \sum_{j=1}^{2} \delta U_{jn} ,$$

$$\delta U_{in} = AU_{in} + H_e^T R H_e V_{in} ,$$

$$\delta V_{in} = -A^T V_{in} + \mu WW^T U_{in} .$$

To make the above procedure numerically stable (note that to get $P_{n+1}$ we have to invert $U_{n+1}$) we employ the reinitialization trick proposed in [3]: namely, we set $V_n = P_n$, $U_n = I$ so that $U_{n+1}$ obtained through (12) is well-conditioned numerically. The advantage of the reinitialized
method over conventional non-reinitialized one is demonstrated by Figure VI. The implicit mid-point method for the state estimator $\hat{x}$ takes the following form.

$$\dot{x} - \frac{h}{2} A x = \dot{x}_n + \frac{h}{2} P_1 h x H R^{-1} Y (t_{n+\frac{1}{2}}) - H x_1 n ,$$

$$\dot{x}_{n+1} = 2 \dot{x} - \dot{x}_n , \quad \dot{x}(t_{min}) = 0 , \quad t_{n+\frac{1}{2}} := t_n + \frac{h}{2} . \quad (13)$$

VII. EXPERIMENTAL RESULTS

In this section we present results of the numerical experiments on source estimation for 2D acoustic and 3D elastic wave equations. Figure 3 represents so-called crash-test describing the case when the assumption about smoothness of the source intensity over time is violated. The simulation was performed for 2D acoustic wave equation and it was assumed that the position of the source is known. So, in fact, the problem of source tracking was solved.

Figure 4 shows the estimation results for the case of 2D acoustic wave equation and given source position when subject to a standard Ricker wavelet source function. The source estimate (bottom left) is almost exact if the receivers are quite close to the actual source location (top left) and there is a time delay in the intensity tracking (bottom right) if the receivers are further away (top right) from the source.

Figure 5 displays the source estimation results for the case of 3D elastic wave equation (top left) and assuming that the source position is unknown but is in either of 3 given locations. The receivers are located close to the source. The algorithm properly identifies actual source location (middle) out of 3 possible locations and tracks the intensity of the source. The other two locations receive low weights (compared to the one in the middle).

The simulations were performed on an IBM Blue Gene/Q using on a grid defined by approximately sixteen thousand $5^{th}$ order elements, resulting in a total of approximately 6.5 million degrees of freedom. The parallelization strategy is based upon decomposition of the grid across multiple processes such that each process contains a unique set of the
global GLL points and hence contiguous rows of the global mass, damping, stiffness matrices. The explicit construction of a stiffness matrix implies that the time marching update can be performed by a distributed matrix vector multiplication at each time step and to to so the implementation makes use of the Watson Sparse Matrix Package (WSMP) in order to provide a scalable code allowing for hybrid parallelization based on multithreading and the message passing interface (MPI).

VIII. CONCLUSION

The paper presents a simple yet powerful source estimation method based on min-max state estimation technique. The approach taken here is hybrid, namely the elastic wave equation is first discretized by using spectral element method, and a source estimator is then derived for the continuous uncertain parameters modelling the projection error. The estimator is discretized by means of the implicit midpoint method which preserves quadratic invariants. Different numerical experiments illustrate efficacy of the proposed technique.

REFERENCES


Fig. 5. An illustration of a sample forward simulation on the SEG/EAGE salt model dataset, illustrating the magnitude of the elastic displacement field and the receiver traces when subject to a standard Ricker wavelet source function, and the source estimates for 3 locations at (4172.67, 500), (4500, 500) and (4827.33, 500). True source is located at (4500, 500). Note the amplitude of the middle plot is much larger than the upper and lower plots.