REGIONAL-SCALE DIFFERENTIAL TIME METHODS: DEVELOPMENT AND APPLICATION TO THE SIBERIA DATA SET

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ABSTRACT

The University of Wisconsin-Madison (UW-Madison) group is developing improved methodologies for regional-scale three-dimensional (3D) seismic tomography, and is working collaboratively with Los Alamos National Laboratory (LANL) and Michigan State University (MSU) on applications of these methods to the Siberia data set assembled by MSU. The tomographic study proposed here will emphasize the accretionary regions to the south and east of the Siberian craton, providing the first detailed 3D look at the seismic structure of continental eastern Russia.

There are four main tasks in this project: (1) an extension of our development of double-difference (DD) seismic tomography to the use of station-pair residual differences, including incorporation of a new method for resolution matrix calculation; (2) testing, refinement, and adaptation of a method for spherical-earth finite-difference (SEFD) travel time calculations for use in DD tomography; (3) an extension of our Cartesian adaptive-grid DD tomography algorithm to spherical coordinates; and (4) collaborative work among the UW-Madison, LANL, and MSU groups to apply these analysis tools to the Siberia data set.

Our work under Task 1 has so far focused on the incorporation and testing of the new resolution matrix calculation method in an existing DD tomography code. The PROPACK package developed by Larsen (1998) is able to efficiently and accurately estimate singular values and vectors for large matrices based on the Lanczos bidiagonalization with partial reorthogonalization (BPRO). We have made substantial progress towards incorporating the PROPACK package into the double-difference seismic tomography code tomoDD, allowing its use to estimate the model resolution matrix for large seismic tomography problems. Compared to previous LSQR-based methods for estimating the model resolution matrix, the PROPACK-based method accurately calculates the full resolution matrix and thus gives a complete description of how well the model is resolved.

Task 2 involves the testing, refinement, and adaptation of a new method for SEFD travel time calculations developed by S. Roecker. The basic concept is the extension of a standard Cartesian FD travel time algorithm to the spherical case by (1) developing a mesh in radius, co-latitude, and longitude; (2) expression of the FD derivatives in a form appropriate to the spherical mesh; and (3) the construction of "stencils" to calculate extrapolated travel times. S. Roecker has developed this code, and we have begun to test it against another existing SEFD code (Flanagan et al., 2000, 2006). We will then integrate it into our DD tomography algorithms.

Our other work planned for Year 1 includes: acquire and enter additional seismic phase data from eastern Siberia into the MSU Siberia data base (MSU); parse newly acquired datasets into NNSA Schema tables (LANL); load and integrate new data from LANL and MSU into the LANL research knowledge base (LANL); advance and apply interstation travel-time distance inversion method for catalog pick quality control to Siberia data set (LANL); develop P and S datasets from LANL research knowledge base for use in DD tomography and participate in the application of DD tomography (LANL); apply new DD tomography algorithms to the Siberia data delivered by MSU and LANL (3 subregions) (UW-Madison).

OBJECTIVES

The UW-Madison is investigating and developing new and improved methodologies for regional-scale three-dimensional (3D) seismic tomography using a combination of event- and station-pair arrival time differences, and is working collaboratively with LANL and MSU on applications to their Siberia data set. The tomographic work proposed here will provide a more reliable velocity model for both the crust and upper mantle of the accretionary regions to the south and east of the Siberian craton. The resulting model will be compared against previous Russian work and interpreted in the context of regional geology. In addition to the high-velocity cratons and low-velocity rift regions, we hope to identify velocity variations associated with the various types of terranes in the Russian northeast and the Mongol-Okhotsk suture zone.

The components of our proposed work are (1) algorithm development and resolution and uncertainty analysis of event-pair and station-pair residual difference inversion techniques, (2) true spherical-earth (SE) finite-difference (FD) travel time calculations adapted for tomographic inversion algorithms, (3) SE adaptive grid seismic tomography, and (4) application of these methods to the MSU and LANL Siberia data set.

Task 1 is an extension of our recent development of double-difference (DD) seismic tomography using event-pair residual differences (Zhang and Thurber, 2003) to the use of station-pair residual differences (Steck et al., 2004; Phillips et al., 2005). The latter is somewhat akin to teleseismic tomography but with the sources contained within the model region. Event-pair 3D and station-pair two-dimensional (2D) inversion algorithms currently exist. By 2D, we mean a 2D "map" of variable Pn velocity, similar to the method of Hearn (1996). We will extend the station-pair inversion to model 3D structure, and we will develop inversion algorithms that include both event-pair and station-pair residual differences, as well as absolute data. We will also carry out a resolution and uncertainty analysis for these algorithms on synthetic datasets, similar to that of Wolfe (2002). We further propose to incorporate an approximate SVD algorithm into the DD tomography code to compute approximate resolution and/or covariance matrices, based on the Lanczos BPRO.

Task 2 involves the testing, refinement, and adaptation of a new method for SEFD travel time calculations. The basic concept is the extension of a standard Cartesian FD travel time algorithm (Vidale, 1990) to the spherical case by developing a mesh in radius, co-latitude, and longitude, expression of the FD derivatives in a form appropriate to the spherical mesh, and the construction of "stencils" to calculate extrapolated travel times. Roecker has developed this code, and we propose to first test it against another existing SEFD code (Flanagan et al., 2000, 2006) and then integrate it into our DD tomography algorithms.

Task 3 is an extension of our recent development of a Cartesian adaptive-grid DD seismic tomography algorithm (Zhang and Thurber, 2005) to spherical coordinates. The technique utilizes extremely flexible tetrahedral model volumes (allowing virtually unconstrained node geometries), sophisticated 3D interpolation methods, and a system for adding or removing nodes based on the density of ray path sampling. The aim is to stabilize the inversion and at the same time maximize the spatial resolution of the inversion. The goal of this task is to adapt the Cartesian algorithm to spherical coordinates by integrating a SEFD travel time algorithm. While this appears to be straightforward in concept, in practice it will be a difficult challenge. We will also develop a new way of adding or removing nodes based on the approximate resolution estimated from the BPRO algorithm in addition to ray sampling density.

Finally, for Task 4, the UW-Madison, MSU, and LANL groups will work collaboratively to apply these analysis tools to the Siberia data set. The applications will be done in different stages, starting with smaller-scale subregions and progressing to the entire region. This effort will provide the first detailed 3D velocity model of continental eastern Russia. We will also generate travel time correction surfaces based on the obtained 3D models that can be used to improve seismic event locations in this region. Finally we will interpret velocity variations in terms of geology and tectonics and attempt a structural regionalization of the study area. Our efforts in Year 1 are concentrated in Tasks 1 and 2.

RESEARCH ACCOMPLISHED

Resolution Matrix Calculation

The primary goal of geophysical inverse problems is to estimate the unknown model parameters from a set of observations. In addition, it is also important to characterize how reliable the resulting model parameters are through a resolution analysis. For smaller problems, the model resolution can be evaluated using a model resolution matrix estimated using the singular value decomposition (SVD) of the sensitivity matrix. For some tomography problems, however, there may be hundreds of thousands to millions of observations and tens to hundreds of thousands of model parameters (Vasco et al., 2003). The SVD algorithm is not practical for such large problems because it requires large CPU memory space and is very time-consuming (Dongarra et al., 1978).

In practice, synthetic tests are generally used to estimate the model resolution and uncertainty by applying the same inversion algorithm to a synthetic data set having the same data distribution as the real data. These synthetic tests include checkerboard test (Humphreys and Clayton, 1988), restoration test (Zhao et al., 1992) and statistical analysis methods such as "jackknifing" and "bootstrapping" (Tichelaar and Ruff, 1989). However, these tests suffer the shortcomings of measuring the sensitivity only with respect to fixed cell or grid patterns (Leveque et al., 1993; Nolet et al., 1999). Soldati and Boschi (2005) contend that the checkerboard test does not provide more valuable information than a simple plot of data coverage. The "jackknifing" and "bootstrapping" methods are computationally very expensive and of questionable use for large tomographic systems (Nolet et al., 1999).

Several researchers have suggested using an LSQR-based method to estimate the model resolution and covariance matrices for large seismic tomography problems (Berryman, 1994a, b; Zhang and McMechan, 1995; Minkoff, 1996; Vasco et al., 1999; Yao et al., 1999; Vasco et al., 2003). LSQR is now a standard algorithm for solving large inverse problems and its core is based on the Lanczos bidiagonalization process (Paige and Saunders, 1982). The central concept of this method is to use Ritz values and vectors resulting from the Lanczos bidiagonalization process to approximate singular values and vectors and then to estimate model resolution and covariance matrices (e.g. Zhang and McMechan, 1995; Vasco et al., 1999). The major argument against using this method is that the Ritz vectors resulting from a limited number of Lanczos bidiagonalization iterations only span a portion of the model space and thus could not provide adequate estimates of model resolution and covariance matrices (Deal and Nolet, 1996; Nolet et al., 1999). However, Yao et al. (1999) contended that although the resolution matrix estimated in this way may not be a good approximation to the full resolution matrix, it is a "full and adequate description" of the properties of the subspace model that the data can actually solve.

Because of the controversies over the validity of the LSQR-based method, the checkerboard resolution test is still the "standard" method to check the reliability of model parameters for seismic tomography applications (Tryggvason et al., 2002), with the exception of a very few studies (e.g. Vasco et al., 1999, 2003; Van Avendonk et al., 2004). The LSQR-based model resolution and covariance matrices estimation is seldom applied in the practical large-scale geophysical inverse problems. Instead, Nolet et al. (1999) proposed an explicit expression for the approximate inverse matrix using a one-step projection method. Although this one-step projection method may give a reasonable estimation of the resolution matrix under some circumstances, i.e. when $\mathbf{AA}^T$ is diagonally dominant (Nolet et al., 1999, 2001), it may fail to approximate the full resolution matrix because it ignores the iterations required to converge in the conjugate gradient method when solving the Penrose condition $\mathbf{AA}^{-1} = \mathbf{I}$ (Yao et al., 2001). One approach to estimate the full resolution matrix is to apply parallel Cholesky factorization to the matrix $\mathbf{A}^T\mathbf{A}$, an approach that is feasible and efficient on shared-memory multiprocessor servers (Boschi, 2003; Soldati and Boschi, 2005). This approach may potentially lose its accuracy since the matrix $\mathbf{A}^T\mathbf{A}$ is more ill-conditioned than the matrix $\mathbf{A}$ and it cannot calculate singular values and vectors that are important to assess the stability of the system.

Recently, a package called PROPACK that can accurately estimate the singular values and vectors for sparse matrices was developed by Larsen (1998). The PROPACK package is still based on the Lanczos bidiagonalization process but it is able to estimate the larger singular values and vectors more accurately. This method is shown to be very efficient for estimating the full model resolution matrix for inverse problems having hundreds of thousands of observations and tens of thousands of model parameters. Using this method, estimating the full model resolution matrix is no longer a significant challenge for large inverse problems.

With the ability of using the PROPACK package to accurately and efficiently estimate the singular values and vectors for a large sensitivity matrix, it is then straightforward to construct the covariance matrix in a similar way to that for estimating the resolution matrix (Aster et al., 2005). Therefore, a strict uncertainty analysis for large geophysical inverse problems is possible, although we note that the solution from the regularized system is biased by the applied regularization methods (Aster et al., 2005).

Preliminary results from applying this approach to a test dataset from Mt. Etna, Italy, have proven successful and provide a number of additional findings. It is generally reasonable to use ray sampling density to describe model resolution in a qualitative manner. Furthermore, the model resolution estimated for just velocity inversion always overestimates that for the true simultaneous inversion, but in a relatively predictable manner. Our results also confirm that the DD seismic tomography method is better able to characterize the source region structure with substantially higher resolution than is obtained via conventional tomography. With availability of the PROPACK package for efficiently estimating the singular values for large sensitivity matrices, we can also easily estimate optimal smoothing parameters for seismic tomography problems.

Spherical-Grid Finite-Difference Travel Time Calculation

The eikonal equation in spherical coordinates is:

$$(dt/dr)^2 + (1/r\ dt/d\theta)^2 + (1/(r \sin\theta)\ dt/d\phi)^2 = s^2 \tag{1}$$

where r is the radius from center of earth, dr is positive away from the center, $|dr| = h$, θ is the co-latitude (0° at North Pole, 90° at the equator), $d\theta$ is positive to the south, $|d\theta| = \Theta$, ϕ is longitude, $d\phi$ is positive to the south, $|d\phi| = \Phi$, and s is slowness.
To solve this system, we must account for the differences in r, θ, and ϕ for each node in the mesh. Thus, for each node i we assign r_i, θ_i, ϕ_i, and also signs for directional purposes. It is then necessary to derive expressions for each of the "stencils" used in the algorithm. For example, for Scheme A of Vidale (1990), the algorithm computes the time at one point given the times at 7 adjacent points (thus 7 of the eight points of a cell are known).

Referring to Figure 1 and Table 1, the FD derivatives are:

$$\begin{aligned} dt/dr &= [(t_4 - t_0) + (t_5 - t_1) + (t_6 - t_2) + (t_7 - t_3)]\ /4 \\ 1/r\ dt/d\theta &= [(t_0 - t_3)/r_1 + (t_1 - t_2)/r_1 + (t_4 - t_7)\ /r_2 + (t_5 - t_6)\ /r_2]\ /4\Theta \\ 1/(r \sin\theta)\ dt/d\phi &= [(t_0 - t_1)/(r_1 \sin\theta_2) + (t_3 - t_2)/(r_1 \sin\theta_1) + (t_4 - t_5)/(r_2 \sin\theta_2) + (t_5 - t_6)/(r_2 \sin\theta_1)]/4\Theta \end{aligned} \tag{2}$$

From these equations, it can be shown that the eikonal equation for this stencil is

$$\begin{aligned} s^2 = &\left[\sum_{i=0}^{7} t_i^2 + 2\sum_{i=0}^{6} t_i g_i \sum_{j=i+1}^{7} t_j g_j\right] \Big/ 16h^2 + \left[\sum_{i=0}^{7} (t_i/r_i)^2 + 2\sum_{i=0}^{6} t_i n_i/r_i \sum_{j=i+1}^{7} t_j n_j/r_j\right] \Big/ 16\Theta^2 \\ &+ \left[\sum_{i=0}^{7} (t_i/(r_i \sin\theta_i))^2 + 2\sum_{i=0}^{6} t_i m_i/(r_i \sin\theta_i) \sum_{j=i+1}^{7} t_j m_j/(r_j \sin\theta_j)\right] \Big/ 16\Phi^2 \end{aligned} \tag{3}$$

This expression can be rewritten in the form $at_7^2 + bt_7 + c = 0$, which is then solved for t_7, given the values for t_0 through t_6. Comparable equations can be derived for the "edge" and "face" stencils of Vidale (1990).

The first step is to validate the algorithm. This will be done by comparing calculated travel times against analytic solutions for simple earth models and against calculated travel times from the sphere-in-a-box code (Flanagan et al., 2000, 2006). In fact, this will provide a valuable validation of the latter code in the process. If we find discrepancies, then we will need to expand the evaluation to include another spherical-earth code, most likely an existing shooting method. Preliminary work indicates that the Roecker algorithm is quite accurate, and is less sensitive to accuracy issues related to grid spacing than the "sphere-in-a-box" algorithm due to the former method's intrinsic spherical geometry.

The second step will be to integrate the SEFD code into the regional-scale DD tomography code (tomoFDD; Zhang et al., 2004). This will require significant coding changes, as the tomoFDD code has an underlying Cartesian system. This step will be time-consuming, but in the end will provide a tremendously valuable tool for regional and even global seismic tomography. The same code can also be used for single- or multiple-event location.

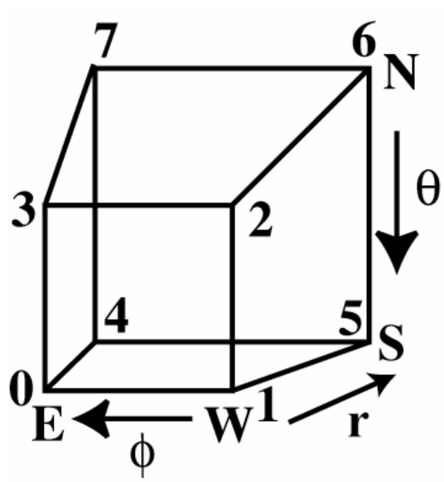

Figure 1. Geometry of a basic cell for the spherical-earth FD calculation of travel times.

Table 1. Convention on point numbering; the signs are the coefficients for the derivatives dt/dr, dt/dθ, and dt/dϕ as shown below.

Point	Position	r	θ	ϕ	r Sign (g)	θ Sign (n)	ϕ Sign (m)
0	Deep SE	r_1	θ_2	ϕ_2	-1	1	1
1	Deep SW	r_1	θ_2	ϕ_1	-1	1	-1
2	Deep NW	r_1	θ_1	ϕ_1	-1	-1	-1
3	Deep NE	r_1	θ_1	ϕ_2	-1	-1	1
4	Shallow SE	r_2	θ_2	ϕ_2	1	1	1
5	Shallow SW	r_2	θ_2	ϕ_1	1	1	-1
6	Shallow NW	r_2	θ_1	ϕ_1	1	-1	-1
7	Shallow NE	r_2	θ_1	ϕ_2	1	-1	1

Other Year-1 work

In addition to the work mentioned above, in Year 1 MSU will acquire and enter additional seismic phase data from eastern Siberia into the MSU Siberia data base. LANL will parse newly acquired datasets into NNSA Schema tables, load and integrate new data from LANL and MSU into the LANL research knowledge base, and advance and apply interstation travel-time distance inversion method for catalog pick quality control to Siberia data set. UW-Madison will apply new DD tomography algorithms to the Siberia data delivered by MSU and LANL. LANL will participate in the application of DD tomography.

CONCLUSIONS AND RECOMMENDATIONS

Although our 3-year project has just begun, we already have some conclusions and recommendations. Our preliminary tests make it clear that the computation of the resolution matrix (and potentially the covariance matrix as well) with PROPACK will be quite accurate, thus providing a practical means for obtaining this fundamental information for large inverse problems. Similarly, the true SEFD algorithm devised by Roecker apparently can achieve excellent accuracy, and likely can do so over a range of scales of spherical models, from regional to whole-Earth. If further testing confirms these preliminary findings, then we would recommend broad adoption of these approaches for resolution and travel time calculations for large-scale problems.

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