Abstract

The D" region, which encompasses the last 300 km or so of the deep mantle (Bullen, 1963), is thought to be both a thermal and a chemical boundary layer, and the site of vigorous dynamic processes. In the last 20 years, many observations have accumulated that clearly set this region of the mantle apart, as the site of heterogeneity at many different scale lengths. Among the most recent findings, most prominent are the evidence for the existence of ultra low velocity zones (ULVZ) that may extend up to 40 km above the CMB and reach 10% in P velocity contrast, the evidence for anisotropy, as well as small scale heterogeneity, and most notably, sharp lateral gradients in S velocity, at least at the border of the two "superplumes" under Africa and under the central, with peak to peak lateral variations of up to 10% occurring over several hundred km or less.

The evidence for strong lateral variations in D" is best addressed by forward waeform modeling approaches that can handle the 1) propagation of seismic body and surface waves in 3D models with strong lateral variations and in spherical geometry, and 2) diffracted waves along the core-mantle boundary. The most promising method at the present time, the spectral element method (SEM), remains very heavy computationally and requires access to powerful supercomputers. To address the study of heterogeneity in particular regions, such as D", Capdeville (2000) developed a hybrid method that couples spectral element computations with a normal mode solution, so that the spectral elements are used only in the target strongly heterogeneous regions. The modal solution provides a fast and precise solution in regions of the Earth in which a model with a spherical symmetry can be considered. The coupling between the two methods is performed through a *Dirichlet to Neumann* (DtN) operator. Recently, this approach has been extended to the case of a heterogeneous shell "sandwiched" between two spherically symmetric shells. While computationally more efficient, this method still has limitations in frequency for applications on a standard Beowulf cluster.

We have assembled a large dataset of Sdiff waveforms from deep earthquakes, sampling the central and northern Pacific ocean, some of which display intriguing features at relatively short periods (less than 20 sec), likely related to strong and localized variations in S velocity. In order to model these observations, we propose to port the CSEM code to the LLNL cluster environment, and perform a series of forward modeling experiments aimed in particular at determining whether lateral heterogeneity or variations in the vertical plane are responsible for the observed anomalies, and whether these originate in D" itself or at some larger height above the core-mantle boundary.

Project Description

Background

The D" region, which encompasses the last 300 km or so of the deep mantle (Bullen, 1963), is thought to be both a thermal and a chemical boundary layer, and the site of vigorous dynamic processes (e.g. Loper and Lay, 1995; Lay et al. 1998, Garnero, 2000). Its structure is believed to hold the key to many yet largely unanswered questions in deep earth geodynamics, such as the ultimate fate of subducting slabs, the origin of hotspots, the amount of bottom heating driving global mantle circulation, electro-magnetic coupling between the core and the mantle, and the nature of chemical heterogeneity in the deep mantle.

Seismologically, D" has long been known for its distinct properties from the overlying lower mantle: early observations at near core-grazing distances implied decreased velocity gradients as a function of depth for both P and S waves (e.g. Cleary, 1974). In the last 20 years, many observations have accumulated that clearly set this region of the mantle apart, as the site of heterogeneity at many different scale lengths. Among the most recent findings, most prominent are the evidence for the existence of ultra low velocity zones (ULVZ) that may extend up to 40 km above the CMB and reach 10% in P velocity contrast (e.g. Garnero and Helmberger, 1996; Garnero and Vidale, 1999), and the evidence for anisotropy (e.g. Vinnik et al., 1989, 1995; Lay and Young, 1991; Matzel et al., 1996; Kendall and Silver, 1996; Ritsema et al., 1998; Russell et al., 1998; Lay et al., 1998; Panning and Romanowicz, 2004), as well as small scale heterogeneity (e.g. Shearer et al., 1998; Wysession et al., 2000), and in particular sharp lateral gradients in S velocity, at least at the border of the two "superplumes" under Africa (Ritsema et al., 1998; Ni and Helmberger, 1999; 2003) and under the Pacific (e.g. Bréger and Romanowicz, 1998; Toh et al., 2003), with peak to peak lateral variations of up to 10% occurring over several hundred km or less. Such strong variations cannot be interpreted in terms of thermal variations alone.

The evidence for strong lateral variations in D" is best addressed by forward modeling approaches. However, present global waveform modeling approaches rely heavily on assumptions of weak heterogeneity. While the forward modeling of travel times of body wave phases sensitive to the base of the mantle, using standard ray methods, provides helpful insights regarding the character of lateral heterogeneity, much information is yet to be gained from the analysis of waveforms. For this purpose, adequate modeling tools are needed that will handle waveform modeling of the 1) propagation of seismic body and surface waves in 3D models with strong lateral variations and in spherical geometry, and 2) diffracted waves along the core-mantle boundary.

Much progress has been made recently in the development of numerical methods adapted to spherical geometry and able to compute waves emanating from a realistic seismic source, reaching, within reasonable computational time, periods of interest for teleseismic studies, making no assumptions on the strength of velocity contrasts, and able to handle interface waves and interface topography. The most promising new method, the spectral element method (SEM), has been introduced in geophysics and applied to the elasto-dynamic equation (e.g. Faccioli et al., 1996; Komatitsch and Vilotte, 1998; Komatitsch and Tromp, 1999).

The spectral element method for the wave equation in spherical geometry was developed at the Institut de Physique du Globe in Paris by J.P. Villotte and his students. It is a method of high order in space using a local polynomial approximation in space and finite differences in time based on a weak formulation of the wave equation. This method combines the advantages of the flexibility of a finite element method with the precision of a pseudo-spectral method (e.g. Komatitsch, 1997) and the corresponding algorithm is also naturally parallelized, making it computationally attractive. The weak form provides an excellent framework for surface and Stoneley waves (it can handle interface topography well), an optimal numerical dispersion, and allows to take into account models with strong heterogeneity. The first application to the global earth has been provided by Chaljub (2000), who developed a clever meshing of the sphere into hexahedra (mapping cubes into the sphere) as well as a technique that allows to increase the mesh size as a function of depth in the sphere ("mortar", Figure 1, e.g. Bernardi et al., 1994), which is crucial in the earth, due to the rapid increase in velocity with depth, in order to minimize computational costs. The weak form with spectral elements adapted to the spherical geometry is able to handle all problems previously mentioned with a high precision. The high performance of the method is based upon the tensorial formulation of the problem which gives a diagonal mass matrix (Komatitsch and Vilotte, 1998; Vai et al., 1999). However this method has a important numerical cost, and, for realistic frequencies (say 15-25 sec), simulations require computers that are not available at the present time.

On the other hand, spectral elements in the whole mantle can be an overkill when one is mainly interested in modeling heterogeneity in a specific shell, such as D", or in the combination of two shells (top and bottom of the mantle). With this in mind, further progress has been recently made by Capdeville (2000), who developed a hybrid method that couples spectral element computations with a normal mode solution, so that the spectral elements are used only in the target strongly heterogeneous regions. The modal solution provides a fast and precise solution in regions of the Earth in which a model with a spherical symmetry can be considered. The coupling between the two methods is performed through a *Dirichlet to Neumann* (DtN) operator (Capdeville, 2000; Capdeville et al., 2002).

This allows one to focus on the target region and extend computations to much higher frequencies than if spectral elements are used for the whole earth, similarly as previously described for the hybrid FD/ray methods, but without the drawbacks of the FD approach.

The program is mainly written in F90 (more than 95%), F77 and **C**. It uses MPI library for the communications between processors. As in finite element methods, the spectral element part of the program is based upon local calculations. Only the gathering phase requires communications between nodes. The mesh is made through the "cubic sphere" transformation: the spherical shell is divided into six regions and each of these regions are mapped to a cube. To decompose the work on p processors, each region is decomposed into p domains of the same size. The coupling between the two methods is performed in the wave number domain. In this domain, calculations do not require any communication. On the other hand the transformation of the displacement field from the spatial domain to the wavenumber domain requires a 2D interpolation that requires communications. On average, the time spent in communications is less than 10% of the whole calculation.

Recently, the SEM/Coupled mode approach (CSEM in what follows) has been extended to the case of a "sandwich" heterogeneity (Capdeville et al., 2003), with two coupling interfaces within the earth. This allows us to isolate a portion of the earth's interior, such as D", and focus on the modeling of heterogeneity in that region, while performing faster mode computations in both the rest of the mantle and the core (Figure 2). It is also possible to extend this approach to consider several such layers (for example including a strongly heterogeneous crust).

Work plan

We have been applying the CSEM approach to investigate how accurate the predictions of tomographic models are for Sdiff waveforms observed at different azimuths from deep sources in the western Pacific ocean (Capdeville et al., 2003). The results indicate, as previously shown from travel time studies (e.g. Bréger and Romanowicz, 1998), that tomographic models do a good job at predicting the sign of the Sdiff travel time shifts, but underestimate the corresponding lateral variations in velocity in D" (Figure 3). They also show that there are strong amplitude anomalies in the observed waveforms that cannot be explained by the current tomographic models, most likely because the gradients in the model are too weak. On the other hand, sSdiff waveforms are poorly modeled by current tomographic models, indicating strong heterogeneity on the source side, near the surface bounce point of the sSdiff. This is also why only deep events are considered so far, in order to limit the effect of source side upper mantle structure on Sdiff.

We have collected a large dataset of Sdiff waveforms across the Pacific Ocean, in order to find optimally sampled areas of D", that, preferably, would be also sampled from different directions of approach, with the goal of adjusting the tomographic model in the deep mantle to better explain the observed time and amplitudes of the Sdiff waveforms. In the course of this work, and in particular while inspecting waveforms as a function of azimuth for particular events, we have found some intriguing waveforms that show unexpected shapes, in particular double peaks (Figure 4) that cannot be explained by source effects or simple 1D structure. Moreover, the observed wave distorsions are consistent from event to event and point to localized effects in the deep mantle (they are not seen on sSdiff waveforms, which, on the other hand, present other features due to upper mantle structure on the source side).

Unfortunately, the details of the observed waveforms are lost when filtering above 17 sec, which is the limit of effective computation on our current BSL Beowulf cluster (32 nodes, 1Gbyte of memory at each node). While CSEM is currently implemented down to 12 sec, it takes a whole week of full cluster usage to compute one D" model, much faster than if the standard SEM was used, but still impractical for the purpose of forward modeling.

We here propose to : 1) port the CSEM code to LLNL super-cluster environment, 2) implement a series of forward modeling experiments to adapt the 3D model to better explain the observed waveforms:

1) We propose to port the CSEM to high-performance computing platforms at LLNL. Specifically we will complie and run the CSEM code on the Multiprogrammatic Capability Cluster (MCR) machine. MCR is the world's seventh most powerful supercomputer (November 2003, www.top500.org) and has 1152 nodes each with two 2.4 GHz Pentium 4 Xeon processors and 4 Gigabytes of RAM (2304 total processors). Benchmark tests show that MCR has a peak performance of 7.6 teraflops. The MCR machine runs the LINUX operating system and porting the CSEM code to MCR can be easily done. We are currently running the SPECFEM3D SEM code, developed by Prof. Jeroen Tromp, on the MCR cluster.

We will validate CSEM simulations with the SPECFEM3D code and evaluate the computational cost reduction provided by the CSEM method.

2) One specific goal of the forward modelling experiments, whether the observed double pulses are due to structure in the vertical direction (quasi-horizontal reflectors) or to strong lateral gradients. In this work, effects of structure in other parts of the mantle will be corrected for using current 3D tomographic models and a mode perturbation approach (NACT, Li and Romanowicz, 1995).

In a second step, once a satisfactory D" model has been obtained for the Sdiff waveforms, we propose to utilize the complete SEM code as available at LLNL, to help constrain upper mantle structure (in the source region and under the stations) and expand the waveform database. Indeed, if we can include strong heterogeneity in the upper mantle, we will be able to include sSdiff data as well as Sdiff data from shallower events. The dataset sampling the Pacific region does not currently benefit from dense array data as have been available in south Africa for the African "superplume". It is thus necessary to consider multiple types of phases to increase D" sampling. As the USArray of Earthscope unfolds, we will be well positioned to exploit the denser station distribution to further refine the 3D central Pacific models.

Proposing team

Prof. Barbara Romanowicz is a senior seismologist at U.C. Berkeley with extended experience in global waveform tomography and the modeling of long period seismograms in a 3D earth using normal mode perturbation theory. She has contributed to the development of asymptotic approaches to construct 3D seismograms and partial derivatives in a 3D earth. In the last 4 years, she has been collaborating with Dr Yann Capdeville (currently at the Institut de Physique du Globe in Paris, France), on applications of the CSEM method to the study of D", as well as on comparing CSEM predictions with those of approximate, but more efficient, asymptotic normal mode approaches. Ms Akiko Toh is a graduate student at the Berkeley Seismological Laboratory. She has been working with Prof. Romanowicz and Dr. Capdeville on putting the CSEM method into practice and has been involved in the waveform data collection. She will be performing the forward modeling experiments.

Dr Yann Capdeville recently joined the Institut de Physique du Globe in Paris as where he holds a research position with CNRS, after years spent at U.C. Berkeley's Seismological Laboratory (BSL) as a Miller Post Doctoral Fellow. Dr Capdeville developed the coupled mode/Spectral Element Method (CSEM) and its "sandwich" version and has been collaborating with Dr Romanowicz and her team in applications of this method to study the D" region. Dr Capdeville will guide the UCB/LLNL team to port the CSEM code to the LLNL computers.

Dr Arthur Rodgers

is a research seismologist within the Ground Based Nuclear Explosion Research Group. He did his thesis work on seismic imaging of the the core-mantle boundary and has experience with waveform modeling. He will help port the CSEM code and He will run the CSEM and SPECFEM3D parallel computer codes on Livermore Computing systems.

This project will enhance collaboration between the BSL at UCB and LLNL. Dr. Rodgers will visit the BSL as needed to discuss technical and scientific issues related to this project. The PI and student will visit LLNL to present this work in a seminar.

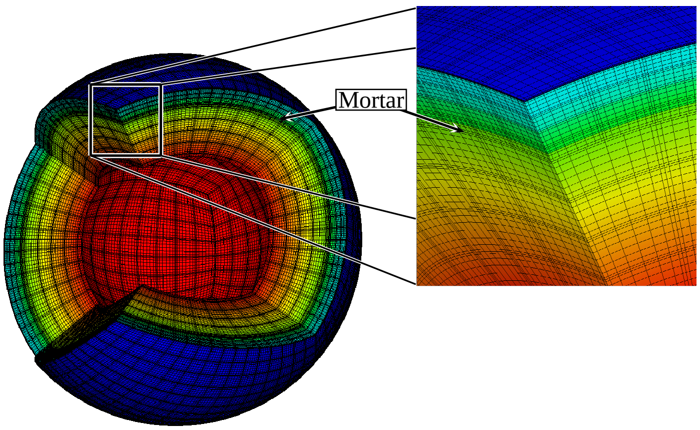

Figure 1: Variable size mesh used for the spectral element method in spherical geometry for PREM (*from* Capdeville, 2000

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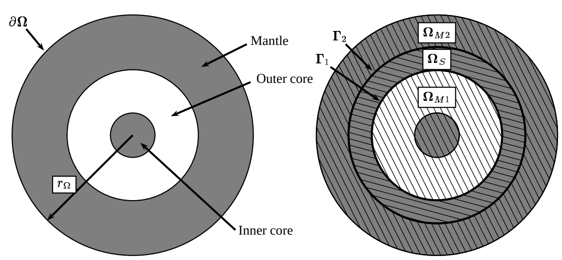

Figure 2: The Earth domain Ω(left) is divided into three parts (right), an external shell Ω_{M2}, an internal shell Ω_S and an internal sphere Ω_M, separated by two boundaries Γ_2 and Γ_1. In our study, Γ_1 is located at the core-mantle boundary and Γ_2 in the lower mantle. We assume that lateral heterogeneities are present only in Ω_S, and use SEM in that domain, and modal solutions in Ω_{M2} and Ω_M, with DtN coupling at the interfaces.

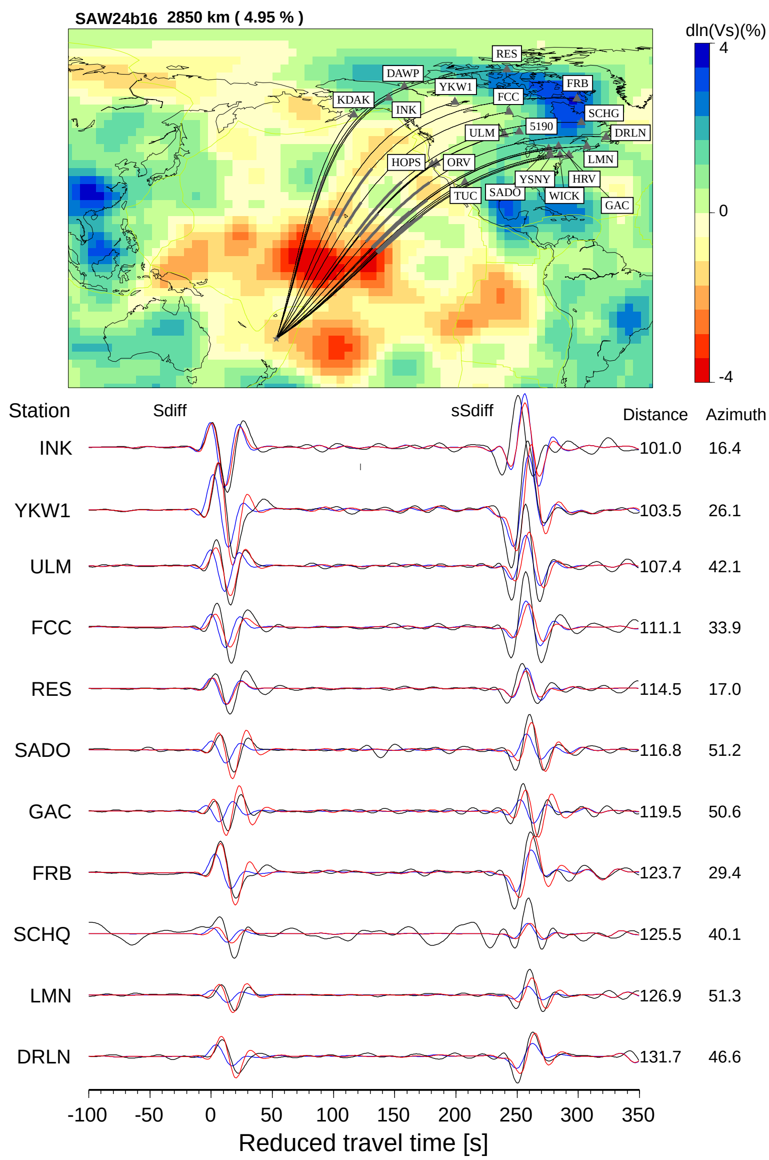

Figure 3: Top: configuration of source and stations for an event in the Fiji island and stations in north America, with portions of paths sampling D" indicated in bold grey. The background model is the SH tomographic model SAW24B16 (Mégnin and Romanowicz, 2000). Bottom: corresponding S and sSdiff waveforms. Black: observed transverse component waveforms filtered between...; Blue: predictions for the PREM model, including ellipticity corrections; Red: predictions of model SAW24b16 obtained using the CSEM computation.

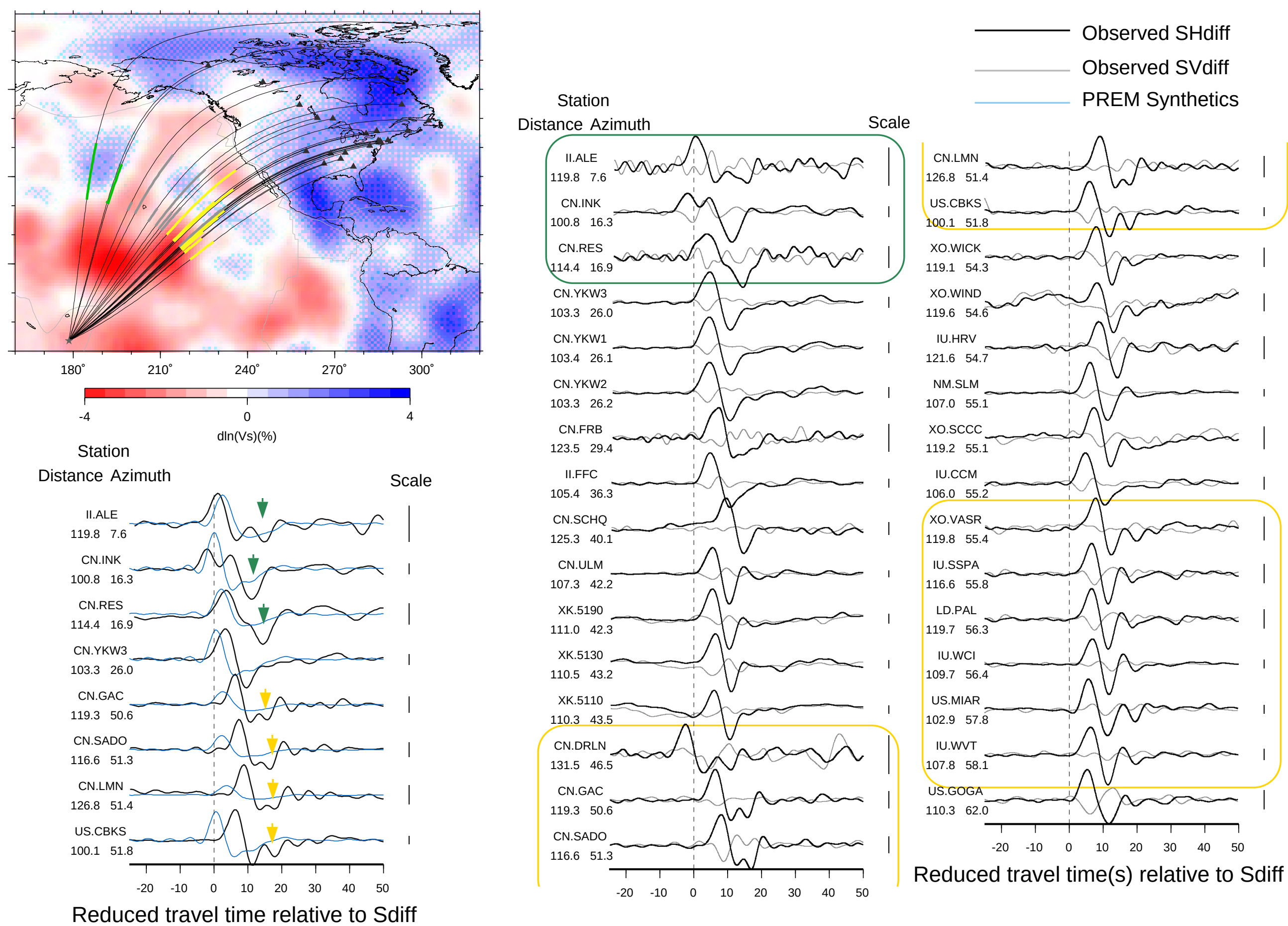

Figure 4: anomalous waveforms

References

Bernardi, C., Y. Maday and A. T. Patera, A new nonconforming approach to domain decomposition: the mortar element method, in *H. Brezis and J. Lions (Eds), Nonlinear Partial differential equations and their applications*, pp 13-51, Pitman, 1994.

Bréger, L. and B. Romanowicz, Thermal and chemical 3D heterogeneity in D", *Science*, **282**, 718-720, 1998

Bullen, K. Introduction to the theory of seismology, 381 pp., Cambridge Univ. Press., New York, 1963.

Capdeville, Y. Méthode couplée éléments spectraux- solution modale pour la propagation d'ondes dans la Terre á l'échelle globale, *Thèse, Université Paris 7*, 2000.

Capdeville, Y., E. Chaljub, J.P. Vilotte, and J. P. Montagner Coupling the spectral element method with a modal solution for elastic wave propagation in global earth models, *Geophys. J. Int.*, **152**, 34-66. 2002.

Capdeville, Y., A. Toh and B. Romanowicz, Coupling spectral elements and modes in a spherical earth: an extension to the "sandwich" case*Geophys. J. Int.*, **154**, 44-57, 2003.

Chaljub, E. Modélisation numérique de la propagation d'ondes sismiques en géométrie sphérique : application en sismologie globale. *Ph. D. thesis, Univ. Paris VII*, 2000.

Cleary, J. R., The D" region, *Phys. Earth. Planet. Inter*, 9, 13-27, 1974.

Faccioli, E., F. Maggio, A. Quarteroni, and A. Tagliani Spectral-domain decomposition methods for the solution of acoustic and elastic wave equations, *Geophysics*, **61:4**, 1160-1174, 1996.

Garnero, Edward J, 2000. Heterogeneity of the lowermost mantle, Annual Review of Earth and Planetary Sciences, 28, 509-537.

Garnero, E. J. and J. E. Vidale, ScP: a probe of ultralow velocity zones at the base of the mantle, Geophys. Res. Lett., 26, 377-380, 1999.

Garnero, E. J. and Helmberger, D. V., Seismic detection of a thin laterally varying boundary layer at the base of the mantle beneath the central-pacific, *Geophys. Res. Lett.*, **23**, 977-980, 1996.

Kendall, J. M. and P. G. Silver, Constraints from seismic anisotropy on the nature of the lowermost mantle, *Nature*, **381**, 409-412, 1996.

Komatitsch, D. Méthodes spectrales et élements spectraux pour l'équation de l'élasto-dynamique 2D et 3D en milieu hétérogène, *Thèse de doctorat de l'Université Paris 7*, 1997.

Komatitsch, D. and J. P. Vilotte, The spectral element method: an effective tool to simulate the seismic response of 2D and 3D geological structures, *Bull. Seism. Soc. Am.*, **88**, 368-392, 1998.

Komatitsch, D. and J. Tromp, Introduction to the spectral element method for three-dimensional seismic wave propagation, *Geophys. J. Int.*, **139**, 806-822, 1999.

Lay, T. and Young, Analysis of seismic SV waves in the earth's penumbra, *Geophys. Res. Lett.*, 18, 1373-1376, 1991.

Lay, T., Q. Williams, E. Garnero, L. Kellogg and M. Wysession, Seismic wave anisotropy in the D" region and its implications, in *The Core Mantle Boundary*, ed. M. Gurnis, M. E. Wysession, E. Knittle, B. A. Buffett,Washington, DC, AGU, 273-298, 1998.

Li, X-D and B. Romanowicz, Comparison of global waveform inversions with and without considering cross branch coupling, *Geophys. J. Int*, **121**, 695-709, 1995.

Loper, D.E. and T. Lay, The core-mantle boundary region, *J. Geophys. Res.*, 100, 6397-6420, 1995.

Matzel et al., Matzel, E. ,M. K. Sen and S. P. Grand, Evidence for anisotropy in the deep mantle beneath Alaska, *Geophys. Res. Lett.*, **23**, 2417-2420. 1996.

Mégnin, C. and B. Romanowicz, The 3D shear velocity structure of the mantle from the inversion of body, surface and higher mode waveforms, *Geophys. J. Inter.*,**143**, 709-728, 2000.

Ni, S. and D. V. Helmberger, Low-velocity structure beneath Africa from forward modeling, Earth Planet. Sci. Lett., 170, 497-507, 1999.

Ni, S. and D. V. Helmberger, Further constraints on African Super Plume Structure, *Phys. Earth Planet. Inter.*, **140**, 2003.

Panning, M. and B. Romanowicz, Mantle flow at the base of the Earth's mantle: evidence from a study of global scale seismic anisotropy, *Science*, **303**, 351-353, 2004

Ritsema, J., S. Ni , D. V. Helmberger, and H.P. Crotwell, Evidence for strong shear velocity reductions and velocity gradients in the lower mantle beneath Africa, *Geophys. Res. Lett.*, **25**, 4245-4248, 1998.

Russell, S.A., T. Lay, and E.J. Garnero, Seismic evidence for small-scale dynamics in the lowermost mantle at the root of the Hawaiian hotspot, *Nature, 396, 255-258*, 1998.

Shearer, P., M. Hedlin and P. Earle (1998) PKP and PKKP precursor observations: implications for the small-scale structure of the deep mantle and core, in The Core-Mantle Boundary Region (M. Gurnis, M.E. Wysession, E. Knittle, and B.A. Buffett, eds), Geodynamics Series, AGU, Washington, DC, 28, 37-56, 1998.

Toh, A., Y. capdeville and B. Romanowicz, Waveform Modeling of 3D Structure of D" Region Using A Coupled SEM/Normal Mode Approach, *EOS Trans A.G.U.*, Fall'03 Meeting Abstract, S31D-0787, 2003.

Vai, R., J. Castillo-Covarrubias, F. Sánchez-Sesma, D. Komatitsch, and J. P. Vilotte (1999) Elastic wave propagation in an irregularly layered medium. *Soil Dyn. Earthquake Eng.*,**18**, 11-18, 1999.

Vinnik, L., V. Farra and B. Romanowicz, Observational evidence for diffracted SV in the shadow of the earth's core, *Geophys. Res. Lett.*, **16**, 519-522, 1989.

Vinnik, L., B. Romanowicz, Y. LeStunff and L. Makeyeva, Seismic anisotropy in the D" layer, *Geophys. Res. Lett.*, **22**, 1657-1660, 1995.

Wysession, M. E., K. M. Fischer, G. I. Al-eqabi and P. Shore, Using MOMA broadband Array ScS-S data to image smaller-scale structures at the base of the mantle, *Geophys. Res. Lett.,* 2000.