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# Simulation of 3D Global Wave Propagation Through Geodynamic Models B. Schuberth, A. Piazzoni, H. Igel, H.–P. Bunge

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**Abstract** This project aims at a better understanding of the forward problem of global 3D wave propagation. We use the spectral element program "SPECFEM3D" (Komatitsch and Tromp, 2002a,b) with varying input models of seismic velocities derived from mantle convection simulations (Bunge et al., 2002). The purpose of this approach is to obtain seismic velocity models independently from seismological studies. In this way one can test the effects of varying parameters of the mantle convection models (MCM) on the seismic wave field. In order to obtain the seismic velocities from the temperature field of the geodynamical simulations we follow a mineral physics approach. Assuming a certain mantle composition (e.g. pyrolite) we compute the stable phases for each depth (i.e. pressure) and temperature by system Gibbs free energy minimization. Elastic moduli and density are then calculated with different equations of state (EOS), depending on the mineral phase. For this we built a mineral physics database based on calorimetric experiments (enthalphy and entropy of formation, heat capacity) and EOS parameters.

# Motivation

- Creation of velocity models independent of seismological observations
- Possibility of testing the effect of various geodynamical parameters on the seismic wave field
- Better understanding of the forward problem of seismology
- Exploration of different processing methods and configurations beyond current observational capabilities

#### Geodynamic Model

- Present day temperature field from mantle convection simulations based on sequential data-assimilation of past plate motions of Bunge et al. 2002
- Whole mantle, spherical geometry
- Over 10 Million finite elements
- $\rightarrow$  ca. 60km horizontal grid spacing
- Rayleigh number based on internal heating of order 10<sup>8</sup>
- Viscosity increases from upper to lower mantle by a factor of 40
- 85% internal heating by radioactive decay
- 15% of heat coming from CMB



#### Conversion of Temperatures to Seismic Velocities - Mineral Physics Model

- Pyrolitic composition (38.53% SiO<sub>2</sub>, 49.64% MgO, 6.31% FeO, 3.29%
  CaO, 2.23% Al<sub>2</sub>O<sub>3</sub>)
- Computation of stable phases by minimizing Gibbs free energy of the system using equation of state parameters and calorimetric data
- Density and elastic moduli obtained by appropriate equations of state (for each phase) and Voigt-Reuss-Hill averaging for the mixture applied to temperatures and pressures from the geodynamic model





Figure 3. Molar fractions of the stable phases at 1800K for a pyrolitic composition from Gibbs free energy minimization.





Figure 2. Radial temperature profile of the geodynamic mantle convection simulation together with the minimum and maximum temperature for each depth.

### Tomography Model S20RTS (CalTech)

- Shear velocity model derived from Rayleigh wave dispersion, body wave travel time and normal mode splitting data
- Parameterized in spherical harmonics up to order and degree 20 and 21 vertical spline functions
- Ref.: J. Ritsema and H.J. van Heijst, Science Progress, 83, pp. 243-259, 2000.

**Pre-Results** At this early stage of the project only



Figure 1. Compilation of Earth models used in this study. a) Temperaure field from geodynamic mantle model. b) Velocity model derived from a) using a mineral physics model. c) Velocity model obtained by linear scaling of dT (from model a) to dvs. d) Tomography model S20RTS for comparison to b) and c)

Figure 4. Elastic properties and density for a pyrolitic mantle for a large range of P and T conditions obtained by applying appropriate EOS for the stable phases.





two simulations have been performed. Figure 5 is showing results using values of  $-0.2 \cdot 10^{-3}$  (Fig. 1c) and  $-0.1 \cdot 10^{-3}$  for  $\frac{dvp}{dT}$  (red and blue seismograms, respectively, values from Duffy & Ahrens, 1992). The green trace is resulting from a simulation using the model S20RTS. One can clearly see the very early arrival times of the S, SS and SSS phase for the simulation using the greater conversion factor (red line).



Figure 5. Tokachi Oki M8.1 Sep. 2003, Transverse Component – Station WET, Germany

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#### Problems to be solved

- Current computation of shear moduli is not yet consistent (at the moment derived from AK135M using  $\frac{G}{P}$  vs.  $\frac{K}{P}$ ). This is due to different depth to pressure relations in PREM and AK135M.
- Rayleigh number in MCM is of order 10 too low which is due to limitations in computer power leading to overestimated temperature variations. In addition, the boundary layers (appr. 200 km) are larger than in reality due to grid resolution.
- Configuration and parameterization for theoretical seismological study are not yet defined (e.g. Events to be simulated, stations, also virtual ones, processing and evaluation of synthetic data).

## How?

- Using appropriate equations of state for shear moduli (done but not yet implemented)
- New Linux cluster will be available end 2005 which will allow us to perform simulations with grid size suited to resolve boundary layers correctly and apply Rayleigh numbers equal to estimates for Earth's mantle
- Due to the problems mentioned, comparisons to seismological (reference) models are not yet feasible.
   → averaging 3D MCM will give theoretical 1D reference model

Concerning seismic analysis and processing discussion and suggestions are welcome.