ERC Advanced Grant 2012
Research proposal (Part B section 2)[1]
(not evaluated in step 1)

Section 2: *The Project proposal* (max. 15 pages, excluding Ethical Issues Table and Annex)
(see Guide for Applicants for the Advanced Grant 2012 Call – Instructions for completing "Part B" of the proposal)

a. State-of-the-art and objectives

1 Preamble

How are deep mantle processes related to the mapped geological record? How can we reconcile geochemical observations with geophysical inferences? These are first order unanswered questions despite our steady progress in imaging the Earth's internal structure and understanding the high temperature and pressure properties of minerals. To make a breakthrough, we have to understand solid-state convection in the Earth's mantle in much greater detail. Much is known about the physical processes, such as melting and the delicate interaction between thermal and chemical buoyancy, but the parameters that enter their mathematical description are not very well known. Once these parameters are determined, the thermo-chemical evolution of our planet can self-consistently be modelled. The state-of-the-art is to roughly estimate these parameters and qualitatively compare the modelling to some relevant geophysical, geochemical or geological observations. This comparison is not comprehensive and never explains all observables. We propose a radically new approach, where all observables are used together to infer these parameters directly, using a fully non-linear Bayesian inference technique based on neural networks. This will determine for the first time the initial conditions at the Earth's formation, the Earth-like flow parameters essential to model the thermo-chemical evolution of our planet and produce models that are simultaneously consistent with the main different geophysical and geochemical datasets.

2 Introduction (state-of-the-art)

Seismology has been quite successful in delineating the downward flow of mantle convection (e.g. Woodhouse and Dziewonski, 1989; van der Hilst et al., 1997; Ritsema et al. 1999) by producing highly consistent images from study to study. There have also been claims of models of a three-dimensional (3-D) return flow (e.g. Montelli et al., 2004), but these images remain quite controversial to date. Despite its success, seismic tomography is hampered by the imperfect coverage of worldwide seismic events and stations. The elastic waves therefore see the Earth's interior unevenly and this is responsible for non-unique solutions of the imaging problem. This can only be remediated by more data coverage. Currently the trend is to merge data with different sensitivity to Earth structure (e.g. Ritsema et al., 2011). Since these data are measured at different frequencies, the classical ray theory is not precise enough and finite frequency kernels should be employed (e.g. Dahlen et al., 2000; Spetzler et al., 2002). Finite frequency modelling is a topical subject in theoretical as well as computational seismology. Theoretical considerations have shown how to calculate these kernels for 1-D reference models only. The tomographic inverse problem is non-linear and therefore these kernels need to be updated in 3-D models. This can only be done numerically. Recently, the necessary computational resources and stable codes have become available to solve the wave equation in general 3-D media. Tromp et al. (2005) showed how to use these exciting new developments to perform such kernel computations with adjoint techniques and first applications on a local as well as a regional scale have just been published (Tape et al., 2009, Fichtner et al, 2009, Fichtner and Trampert, 2011). Gravity data in combination with density variations inferred from seismic tomography have provided major constraints on the radial viscosity structure of the mantle (e.g. Hager et al. 1985; Forte and Mitrovica, 2001); we will also use such data here. Heat flow distributions (e.g. Pollack et al., 1993; Davies and Davies, 2010) are also a major constraint, particularly in oceanic areas where they constrain the age distribution of oceanic lithosphere (Parsons, 1982).

Mineral physics is essential for the interpretation of seismic tomography. Indeed, if we know the elastic properties of all candidate minerals of the Earth's interior, we can calculate the velocities for any desired mixture, pressure and temperature. Comparing such calculations to images from seismic tomography then provides invaluable information on the current thermo-chemical state of the Earth's deep interior. Ideally,

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[1] Instructions for completing Part B section 2 (B2) can be found in the Guide for Applicants for the Advanced Grant 2012 call. For specific information about financial issues, please consult the Guide for ERC Grant Holders on the ERC website.

such elastic properties should be determined at all pressures and temperatures for all minerals relevant for the Earth. Although much progress has recently been made on the experimental (Bass, 2007) as well as the theoretical side (Alfe, 2007), many relevant temperature and pressure ranges remain unexplored, and as a consequence we rely on extrapolations based on equations-of-state (EOS). Since the pioneering work of Birch (1952), many EOS have been proposed (e.g. Trampert et al., 2001; Deschamps and Trampert, 2004), but the self-consistent approach recently developed by Stixrude and Lithgow-Bertelloni (2005, 2011) is superior to all others. Elastic data for most of the 30 mineral species, which constitute the major element composition of the Earth's mantle, are well determined in some temperature and pressure range and can be used in conjunction with the self-consistent EOS. Topical subjects mineral physics community are the exact properties of the recently discovered post-perovskite phase (Murakami et al., 2004; Oganov and Ono 2004), the effect of water on transition zone minerals (e.g. Litasov et al., 2006) and iron partitioning in the lower mantle (e.g. Irifune et al., 2010).

Trace element geochemistry adds considerable independent constraints on mantle heterogeneity and evolution. Noble gases and other elements offer distinctly different types of constraints as reviewed, for instance, in Hilton and Porcelli (2003) and Hofmann (2003), respectively. To explain the data, at least four chemically-distinct end members are needed, which are variously interpreted to be primordial, or recycled. With ever increasing refinement of the measuring techniques, more and more isotope systems can be analysed, which often challenge existing interpretations and require additional complexity or end members to explain. Traditional interpretations of geochemical data involving compositionally-distinct layers are in conflict with the whole mantle convection that is typical inferred from geophysical data (for a review see Tackley, 2007), which over the years has led to a heated discussion on how to unify geophysical and geochemical evidence on mantle structure and evolution. One reason for the discrepancy is that all proposed models only consider subsets of the available data, but the major reason is that geophysical models are based on major element chemistry, while geochemistry as a field is mainly analysing minor or trace elements. To date no satisfactory way of combining these two complementary approaches has been proposed.

A fundamental but unanswered question is whether the driving forces of mantle convection are purely thermal (e.g. Schuberth et al., 2009) or have a compositional component (e.g. Deschamps and Tackley 2009). A recent attempt to discriminate between thermal plume clusters or thermo-chemical piles in the lowermost mantle concluded that seismic velocity models alone cannot distinguish between these modes of convection (Bull et al., 2009). While many thermal convection studies with various degrees of complexity have been conducted over the last 40 years (e.g. Schubert et al. 2001), thermo-chemical flow models are computationally more challenging, particularly in three dimensions (3-D). After a number of 2-D or 3-D cartesian studies in the 1980s and 1990s (e.g. van Keken et al, 1997; Tackley 1998), 3-D spherical studies emerged in the 2000s using three numerical codes: CitcomS (e.g. McNamara and Zhong, 2004), TERRA (e.g. Oldham and Davies, 2004) and StagYY (Nakagawa and Tackley, 2008; Tackley, 2008). Although the Earth contains many different minerals, 3-D global studies to date have been limited to two chemically distinct materials, which, however, does appear to be enough to explain the observed long wavelength heterogeneity of the Earth's mantle (Deschamps et al. 2007). Such calculations require many input parameters (Rayleigh number, viscosity law, chemical density contrasts, fraction of primitive material, Clapeyron slopes of phase transitions, concentrations of radiogenic and other trace elements, …) many of which have large uncertainties for the Earth.

3 The challenge

Seismology is crucial in a multi-disciplinary effort to understand mantle dynamics and provides us important clues to the causes of mantle flow. In flow calculations, however, the driving forces are density variations while seismology most readily provides wave speed variations. Due to early successes in interpreting tomography and the geoid (Hager et al., 1985), it is often assumed that wave speed and density variations scale with one another, which means that temperature variations are causing both density and wave speed variations. This has led to a vast research field of computer simulations of mantle flow using purely thermal models (Schubert et al., 2001). There is, however, increasing evidence that major element variations play an important role in understanding tomography (Ishii and Tromp, 1999; van der Hilst and Karason, 1999, Resovsky and Trampert, 2003). The key to unravel temperature from compositional variations is a precise mapping of density variations (Trampert et al., 2004), but it remains a challenge. The mapping of the density variations with the same resolution as wave speeds variations will be fully addressed in this proposal.

Most elastic parameters of all major minerals are known to a good precision and together with a self-consistent thermodynamic description allow us to predict seismic wave speeds and density at a given temperature and pressure (Stixrude and Lithgow-Bertelloni, 2005, 2011). The difficulty is to know how to parameterise the Earth. Should we use oxides, minerals or rocks? Should we make equilibrium assemblages, minimizing the Gibbs free energy, or make simple mechanical mixture by Voigt-Reuss-Hill averaging scheme? These choices are very important for the interpretation of seismic tomography (Ritsema et al., 2009) or for the style of mantle convection (Nakagawa et al., 2010). This parameterisation issue, the main obstacle for linking seismology and geodynamics, will also be fully addressed in this proposal.

Tracking of trace elements has been included in a number of mantle convection studies, either to look at the evolution of noble gases (He and Ar) or to look at recycling of isotopes like U and Pb, but never both simultaneously. The most sophisticated of these models include fractionation of different elements by melting that produces crust, and partitioning of each isotope between melt and solid. In this way, trace-element and major-element chemistry is coupled. Using such an approach, Christensen and Hofmann (1994) demonstrated that a layer with a HIMU (high U/Pb) signature can build up above the CMB by segregation of subducted crust, but the correct isotopic age was only obtained if the model was run for 3.6 Gyr rather than the full 4.5 Gyr. Using a model with similar approximations (Xie and Tackley, 2004b) found that the best explanation for the age paradox is a change in subduction environment 2.0-2.5 Ga ago, with HIMU not being produced before this time. Higher Rayleigh numbers were found to produce less basalt segregation by Brandenburg and van Keken (2007). Including the additional isotopes Sm-Nd, Rb-Sr and Re-Os, Brandenburg et al. (2008) found that melting in both mid-ocean ridge and continent production environments is necessary to produce realistic geochemical signatures in all of these systems.

For noble gases, passive mixing and outgassing was tracked in a series of studies (van Keken and Ballentine, 1998, 1999; van Keken et al., 2001), but these did not address the cause of high ^{3}He/^{4}He ratios observed in some ocean island basalts. By tracking the evolution of He isotopes caused by melting and crustal recycling, Ferrachat and Ricard (2001) and Xie and Tackley (2004a) found that high ^{3}He/^{4}He ratios can be caused by recycling, consistent with some geochemical arguments (Albarède, 1998; Anderson, 1998; Class and Goldstein, 2005). On the other hand, the models of Samuel and Farnetani (2003) showed that the alternative possibility of high ^{3}He/^{4}He originating in a primordial dense layer is also dynamically viable, so the matter is still under debate.

Thus, tracking trace elements in thermo-chemical mantle convection models is a well-established technique, but previous models have a number of limitations. None have simultaneously reconciled noble gas signatures with the constraints from other isotope systems. None have taken into account effects due to melting of a heterogeneous source region (e.g. Ito et al., 2008; Phipps Morgan, 2001). None have included "internal differentiation" caused by partial melting that does not produce crust, such as a basal magma ocean above the CMB (Labrosse et al., 2007), due to high water content as material leaves the transition (Bercovici and Karato, 2003), and in the deep upper mantle in the early Earth (Lee et al., 2010). Perhaps most importantly, none have simultaneously tried to reconcile geochemical constraints with geophysical constraints from seismology, gravity and heat flow. We propose to address these important issues in this proposal.

A variety of thermo-chemical models have been proposed in recent years, but whether or not they represent the Earth is an unresolved first order question. All models explain some features of the Earth, but a coherent dynamic understanding is currently lacking. This integrated understanding is the main challenge addressed in this proposal. The problem is how to compare results of convection modelling to structures found by seismic tomography, gravity, heat flow or geochemical measurements. The flow models are constantly evolving over time. Some geochemical data have time constraints, while geophysical data can be seen as instant snapshots, or boundary conditions, at the present time. While one approach is to run convection models until a certain steady-state regime is observed, other studies have modelled Earth's 4.5 billion year time evolution. The temperature and compositional fields are then converted to wave speed variations using partial derivatives from mineral physics and compared to seismic tomography models. This comparison is mostly based on power spectra of heterogeneity and is exclusively qualitative (e.g. Bull et al., 2009). Deschamps et al. (2007) pointed out the importance of comparing to the density field rather than the wave speed field. Such an approach can identify successful input parameters to convection models but no systematic identification has been done to date. An interesting recent development is to run flow calculations in the adjoint mode (Bunge et al., 2003). Using techniques of data assimilation, it is then possible to determine the initial conditions (e.g. Liu et al., 2008). We propose for the first time, to use pattern recognition techniques to directly infer the flow parameters compatible with all data without having to use cumbersome adjoint calculations.

4 The project

The work is organised in three work packages: 1) conditioning the observables also referred to as data, 2) the geodynamics calculations and 3) the design of the neural networks linking the flow models to the observables. Appropriate data with sensitivity to the Earth's dynamics need to be selected. While gravity (http://icgem.gfz-potsdam.de/ICGEM), heat flow (http://www.heatflow.und.edu) and geochemical data (http://georoc.mpch-mainz.dwdg.de, http://www.petdb.org) are readily available, a seismic model needs to be developed to incorporate density variations. Flow models incorporating trace and major elements will be produced for many different input parameters (Rayleigh number, viscosity law, chemical density contrast, fraction of dense material, Clapeyron slopes of phase transitions, radiogenic heating concentration…), will track selected trace elements and include chemical differentiation. At regular time steps, geophysical and geochemial observables will be calculated and used as training sets for neural networks to associate the observables with the input parameters. Once trained, we will show the network the data inferred or observed for the real Earth and thus obtain the parameters, which naturally explain these data. Neural networks are a flexible tool, which associate a probability density function to each parameter of interest, taking into account the full non-linearity of the problem without iterative perturbations (Meier et al. 2007). Using mixture density networks, they also provide a natural way of assessing the reliability of each inferred parameter due to the limited sensitivity of the data and their respective uncertainty.

5 Deliverables and impact

This proposal will push current numerical advances to new dimensions and provide a fully integrated understanding of geophysics and geochemistry in terms of thermo-chemical flow models. To our knowledge this is the first attempt to directly infer Earth-like input parameters for convection modelling. This knowledge will allow us to investigate the Earth's thermo-chemical evolution over geologic times based on flow models that are fully compatible with our record of geophysical and geochemical data. The proposed work is central to one of the 25 unanswered scientific questions proposed by Science in its 125 anniversary issue (1 July 2005), to several of the seismological grand challenges (Forsyth et al., EOS, AGU, 13 Oct 2009), to two of the 10 grand research questions concerning the origin and evolution of the Earth identified by National Academies (2008, http://www.nap.edu/catalog/12161.html) and to the focus areas of Utrecht University and ETH. The main deliverables will be:

i. A new fast technique for full long period waveform inversion in the frequency domain

ii. A new 3-D model for wave speeds and density

iii. A database of thermo-chemical flow models for largely varying input parameters.

iv. A database for geophysical and geochemical data with high sensitivity to mantle flow

v. Probability density functions of input parameters for thermo-chemical convection modelling of the Earth

vi. New constraints on evolution of the 3-D distributions of temperature and composition in the mantle

4 PhD Students and 2 postdocs will work in a dynamic group guided by PI Prof. Trampert (UU) and senior team member Prof. Tackley (ETH) and be confronted with state-of-the-art high performance computing and theoretical developments giving them ample and diverse job opportunities in the future.

b. Methodology

1 Observational work package: conditioning of the data for inference

Gravity maps (e.g. Lemoine et al., 1998) and heat flow maps (e.g. Davies and Davies, 2010) are readily available. Under which form we will use those data (slops of spherical harmonic power spectra, regional averages, distributions, …), will be determined in the neural network package, where we will analyse the sensitivity of the data to flow parameters. Many more recent gravity and heat flow data are available in global data repositories (http://icgem.gfz-potsdam.de/ICGEM, http://www.heatflow.und.edu), and those will of course be used for the final inference. The observables containing most information on flow dynamics are the density variations inside the Earth. Those can be obtained from seismic tomography, but because the approximations in existing models are too severe, it is the emphasis of this work package. The geochemical data are also freely available in online databases (http://georoc.mpch-mainz.dwdg.de, http://www.petdb.org), and we plan to use statistical attributes derived from them regionally or globally. Again this will be analysed in detail in the neural network package.

An unbiased estimation of the 3-D density structure is essential to separate thermal from compositional effects (Trampert and van der Hilst, 2005). While geodynamic observables provide some information (e.g. Forte and Mitrovica, 2001), long period seismic data are most suitable. Any waveform inversion technique needs the capability to calculate synthetic seismograms in a 3-D Earth model. Most global codes rely on the code spectral element method (e.g. Komatitsch and Tromp, 2002), which holds exiting prospects for the near future. However, this technique is not suitable for our purposes. The gravitational restoring force provides the high density sensitivity in long period seismograms, but gravity in the spectral element code is incorporated using an approximation, which can bias the calculation of the longest period components. For this project, the best choice is full coupling normal mode theory, developed by Woodhouse (1983). The idea is to use the complete set of modes from a 1-D Earth as a basis for the 3-D Earth. This can be achieved by diagonalizing a coupling matrix, which describes the interaction between all the modes. For all modes below 3 mHz, this matrix is of the size (2347 x 2345) and the problem can be solved on a single processor in a couple of hours (Deuss and Woodhouse, 2001) and on a computer cluster in a fraction of that time. Synthetic seismograms are then easily calculated from the eigenvalues and eigenvectors of the coupling matrix and a source vector describing the earthquake (CMT solutions from http://www.globalcmt.org).

Full coupling theory is essentially exact for any deviation from the original model, except when the shape of the original sphere is changed. We will have to incorporate the effect of Earth's topography. We are only interested in the long wavelength structure, which is best suited for comparisons to global flow models. We therefore limit the modes to less than 3 mHz, and the Earth will be parameterized laterally with spherical harmonics up to degree 12 and vertically with 20 splines maximum. The Earth's topography will therefore be implemented by first order perturbation (not exact), but we don't expect this to be a major problem for modes below 3 mHz.

To use normal mode seismograms for full waveform inversion, we will implement the adjoint method (e.g Fichtner and Trampert, 2011), which proved so successful with the spectral element method. In this approach, the Earth structure is updated iteratively, and at each step the partial derivatives (sensitivity of the seismograms to changes in the model parameters) are recalculated in the latest Earth model. This sensitivity updating correctly treats the non-linearity between the data and the model parameters. It can be shown (e.g. Liu and Tromp, 2008) that, to obtain the partial derivatives, exactly one forward and one backward simulation in time is needed. The interaction between the forward and the backward field provides us the necessary derivatives. It is interesting to note that the magnitude of the derivatives strongly depends on how the data are compared to the calculations (i.e. definition of the misfit function). The free choice of the misfit function can therefore be exploited to maximise, for instance, sensitivity to density variations. We will therefore test many different misfits (e.g. Bozdag et al., 2011) to optimize the imaging of the parameters of interest.

Although such a complete imaging code does not yet exist, all the ingredients individually do. It is therefore straightforward for a PhD student to assemble all the pieces. The full normal mode coupling theory is nicely summarized in Woodhouse and Deuss (2007), with all the references to the formulae. Deriving the adjoint force will follow the method of Liu and Tromp (2008) and Fichtner and Trampert (2011). We have all the necessary computational competence here in Utrecht (see http://www.geo.uu.nl/~jeannot) to produce a code for the partial derivatives. This part will then be integrated in our existing conjugate gradient optimization software. The method will be applied to long period seismograms of all available large earthquakes recorded worldwide (http://www.iris.edu/dms/dmc/).

The software package for full waveform inversion using full normal mode coupling theory will be complementary to the existing and highly used spectral element package. We will similarly make our package freely available to the international community.

- Supervisor: PI
- Support for one PhD student is requested for this part of the proposal
- Deliverables: i and ii
- Resources: Dedicated high-performance computer cluster requested by this proposal, existing inversion software, published theory
- Novelty: Waveform inversion using full normal mode coupling theory together with the adjoint technique

2 Geodynamics work package: producing the flow models for training

This section describes the proposed modelling of coupled mantle convection and geochemistry. This builds on the considerable experience of senior team member Paul Tackley and his coworkers in the field of thermo-chemical mantle evolution (e.g. Nakagawa et al., 2010; Tackley, 2007; for a full publication list see http://jupiter.ethz.ch/~pjt/bibliography.html) and trace-element isotopic modelling (Xie and Tackley, 2004a, b), as well as taking into account other recent works on mantle trace-element evolution and signatures (e.g.

Brandenburg et al., 2008; Ito and Mahoney, 2006; Kellogg et al., 2007). Geochemist Prof. Tim Elliott of Bristol University will be a consultant on geochemical aspects; he and Prof. Tackley are already collaborating within the Marie Curie network Crystal2Plate (http://www.gm.univ-montp2.fr/CRYSTAL2PLATE/home.html).

Physical and major-element model

The mantle is assumed to be an infinite Prandtl number fluid with strongly variable viscosity that is compressible using the compressible anelastic approximation, as is common (e.g. Deschamps and Tackley, 2009; Nakagawa et al., 2010). The geometry will be spherical: either a full 3D spherical shell or a spherical annulus (Hernlund and Tackley, 2008). The main features our physical model (many of which are already implemented in our modelling software outlined below) are:

- Compressibility, the most important influence of which is in the depth- (pressure-) dependent physical properties like thermal expansivity and thermal conductivity, which have been shown to be important in a number of papers since the 1990s (for a review see Schubert et al., 2000).
- A realistic variation of viscosity with temperature, with activation enthalpy (as a function of pressure) H(p) set to values obtained from laboratory measurements or ab initio calculations. This contrasts with the greatly reduced temperature-dependence used in most global mantle convection models. Depth-dependence of viscosity naturally arises from the combination of H(p) with the geotherm but viscosity jumps may occur due to phase transitions; here we propose to include a viscosity jump across the transition to perovskite (at ~660 km depth), which appears to be a robust feature needed to match the geoid.
- Plastic yielding of the lithosphere, which is necessary to facilitate plate tectonics in calculations with strongly temperature-dependent viscosity (e.g. van Heck and Tackley, 2008).
- Continents, as compositionally-distinct entities that can have different physical properties (Rolf and Tackley, 2011).
- A free surface, which appears to greatly improve the realism of self-consistently forming subduction zones by making them single-sided (Crameri et al., 2012).
- Variations in both major-element and trace-element composition. Major element compositions we plan to include are MORB, harzburgite, continental crust and primitive iron-enriched material (initially in the deep mantle). We will also track various trace element isotopes as discussed below.
- Partial melting, which causes differentiation of both major- and trace-elements. The melt fraction is calculated based on comparing the local temperature to the solidus; latent heat is taken into account in the energy equation. Melt produced in the upper ~300 km is assumed to erupt immediately to form oceanic crust, but deeper melt remains molten and may migrate according to Darcy's law (e.g. Hernlund and Tackley, 2007).
- Solid-solid phase transitions that depend on bulk composition. We will try two different treatments (i) a simplified parameterisation in which the main phase transitions in the olivine and pyroxene-garnet systems are individually inserted, and (ii) a self-consistent treatment in which phase assemblages and the resulting physical properties are calculated self-consitently as a function of temperature, pressure and composition (Nakagawa et al., 2009, 2010).
- A cooling core, using well-established energy balance equations.
- Geoid calculation, including self-gravity.

The modelling software StagYY, developed by P. Tackley (Tackley, 2008), will be used and further developed for this purpose. StagYY is the latest development of a modelling code developed in the early 1990s and used for tens of modelling studies. It is based on a finite volume discretization (using the Yin-Yang spherical mesh) and uses a multigrid solver to efficiently obtain a velocity-pressure solution at each time instant. Composition is tracked using tracers (a.k.a. markers, particles) (Tackley and King, 2003). It is parallelised using MPI and can run on up to 1000s of parallel cores with up to billions of unknowns.

Isotope geochemistry model

The basic techniques for including trace-element evolution in mantle convection simulations are well established (e.g. Brandenburg et al., 2008; Christensen and Hofmann, 1994; Xie and Tackley, 2004a, b).

Here we build on previous work by simultaneously considering noble gases and heavier isotopes for the first time, and by considering the influence of sampling processes and "internal differentiation". As in these previous models, trace element evolution is coupled to major element evolution through melting. When (batch) melting occurs, trace elements partition between melt and solid. If the melt is generated above a certain depth (above which melt is buoyant), it is assumed to erupt immediately to form crust. If below this depth, it does not erupt but may migrate relative to the solid (according to Darcy's law), and will be assumed to remain in chemical equilibrium with the surrounding solid. Trace elements in solid material are advected with the flow. Key features of our trace-element geochemistry model are:

- **Trace elements**. We aim to simultaneously satisfy constraints from noble gases and from other systems, in contrast to previous convection studies that focused either on the noble gases He and Ar (van Keken et al., 2001; Xie and Tackley, 2004a) or the U-Th-Pb and Sm-Nd systems (Christensen and Hofmann, 1994; Xie and Tackley, 2004b) but not both. The Rb-Sr and Re-Os systems were additionally considered by (Brandenburg et al., 2008). We will focus on the systems that are mainly influenced by mantle cycling, i.e. U-Th-Pb-He, Re-Os and K-Ar. These give different constraints: for the first two systems, pseudo-isochrons are a major observation, while Ar gives a constraint on the total mantle outgassing and its timing, and 3He/4He indicates the need for two distinct endmembers, the one with the higher ratio being sampled at some hotspots. We will include Sm-Nd and Rb-Sr systems, although it is thought that these are mostly influenced by continental crust extraction (Brandenburg et al., 2008; Kellogg et al., 2002). Additionally we will track water, as discussed below.
- **Major-element compositions**. All experiments will involve differentiation along the MORB-harzburgite trend. In some experiments we will also include (as an initial condition) a primordial layer above the CMB. This is a commonly-cited location for storing incompatible trace elements that are inferred to be "missing" from the MORB source region, including the high 3He/4He endmember (e.g. Deschamps et al., 2011), although there is much debate about its necessity. Additionally, extraction of trace elements into the continental crust is thought to be an essential process for explaining some isotopic ratios, particularly the Rb-Sr and Sm-Nd systems (Brandenburg et al., 2008; Kellogg et al., 2007). Thus, we will perform some experiments including extraction of trace elements into continental crust. Due to the complexity and uncertainty in how continental crust actually forms, this will be parameterised following these studies.
- **Sampling**. The trace-element signature of extracted magma may be different from the trace-element signature of the source region, due to preferential sampling of fertile heterogeneities as a result of their lower melting temperature (Ito and Mahoney, 2005a, b; Katz and Rudge, 2011; Phipps Morgan, 2001). Despite this, the previous convection+geochemistry studies have simply averaged isotopes over some sampling region with a chosen lengthscale (for example 30 km in Kellogg et al., 2007). Thus, we intend to include sampling effects by including different solidii for the different major-element lithologies, similar to the method of (Ito and Mahoney, 2005a).
- **Internal differentiation**. Not all partial melting results in the formation of crust; it can instead serve to fractionate trace elements within the mantle, and several recently-proposed concepts for explaining Earth's trace-element geochemistry have used this basic idea. In the "Transition Zone Water Filter" hypothesis (Bercovici and Karato, 2003), a high water concentration in the transition zone causes partial melting of material upwelling through 410 km, removing incompatible trace elements and trapping them in the transition zone. In the "Basal Magma Ocean" hypothesis (Labrosse et al., 2007), partial melt has existed above the CMB since the earliest Earth, acting as a repository for incompatible trace elements. Other authors have noted the possibility of partial melting and associated differentiated products in the upper mantle (Davies, 2010; Lee et al., 2010). Such mechanisms will be included in our model in a natural manner by partitioning trace elements between melt and solid as usual, but simply not removing the melt. Additionally, water-dependent melting (e.g. Katz et al., 2003) and water cycling will be necessary ingredients.
- **Water cycling**. Water is a very important trace element that has a strong influence on melting as well as physical properties such as viscosity, so tracking its cycling between the surface environment and the deep mantle is important. Unfortunately, understanding how much water can be transported by slabs into the transition zone is difficult because it depends on a complex sequence of phase transitions that depend on temperature and pressure (Ruepke et al., 2004) and requires more detailed modelling than possible at a global scale. Thus we will develop a parameterisation of water transport and loss that depends on the (p,T) conditions (path), and use this to selectively de-water tracers representing subducted crust, as they sink into the upper mantle. Related to this is whether Pb is

subducted or leaves the slab into the mantle wedge region, which is a thought to be an important mechanism for fractionating Pb from U and thereby creating the HIMU endmember since 2-2.5 Ga ago. (Kellogg et al., 2007; Xie and Tackley, 2004b). Considerable expertise in detailed slab modelling and water transport exists at ETH with professors T. Gerya and J. Connolly, and they will act as consultants about these issues. Water degassing and ingress into slabs will be straightforward to implement.

Proposed experiments

While it may seem that there are many input parameters to the model, most of these will be fixed at preferred values while a few will be varied over reasonable ranges. Nevertheless, this requires running a large number (1000s) of numerical experiments, in order to get a reasonable statistical sampling of the parameter space. Models will be run for 4.5 billion years starting with either a chemically homogeneous condition, or one with initial chemical layering. The main physical parameters to vary will be: the reference viscosity (i.e. at some temperature and pressure, also giving a reference Rayleigh number) and viscosity increase at 660 km, the relative density of different bulk compositions in the deep mantle (MORB, primitive material, harzburgite), the plastic yield stress (effective friction coefficient) of the lithosphere and initial CMB temperature. The main geochemical parameters to be varied are initial concentrations of different isotopes (particularly when an initial primordial layer is present) partition coefficients, the extent to which isotopes are extracted into the continental crust, and aspects related to water transport in subduction zones.

The main model outputs, which will be used to train the neural networks, are: distribution of seismic velocities (spectra and amplitude as a function of depth), surface heat flux and its distribution (which gives information about the age distribution of oceanic lithosphere), geoid spectrum and spectrum of admittance ratios, and trace element distributions in erupted basalt. For erupted basalt, we will distinguish between volcanic environments spreading-centers, subduction zones, and intra-plate volcanism. By running 1000s of models, we will build up a database of thermo-chemical convection models for Earth.

Timing and technical development

Although many of the necessary aspects are already implemented in StagYY, considerable code development will be necessary to for the trace element part, including water transport, composition- and water-dependent melting, etc. Additionally, in order to better resolve key regions such as subduction zones and the CMB region in a global model, we plan to implement adaptive mesh refinement (AMR) into the numerical scheme, giving the ability to refine the grid locally, which will require considerable programming effort. We request an experienced postdoc who will work mainly on the necessary technical development, and two staggered PhD students who will perform scientific studies in close collaboration with team members at Utrecht.

- Supervisor: P. Tackley and PI
- Support for 2 PhD students and 1 postdoc are requested for this part of the proposal
- Deliverables: iii
- Resources: Dedicated high-performance computer cluster requested by this proposal, enhanced version of existing modelling software StagYY, existing theory
- Novelty: Advanced convection modelling including all major physical and chemical (major- and trace-element) processes

3 Neural network work package: learning the connections

To link the observables with the various flow calculations, we propose a radically new approach based on neural networks. They can be seen as non-linear filters or basis functions, depending on the application. They are very common in speech, handwriting and pattern recognition. Because they are mostly used in labelling problems, where there is no explicit physical theory linking observations and model, they acquired a bad reputation amongst physicists. The basic idea is to use a training set where the link between input and output is known (e.g. a voice recording and the corresponding word). This set is used to train a neural network which can then be used on new voice recordings to identify the spoken words. It is true that in this particular example, no explicit physical theory links the sound of a human voice and the actual word, in seismology, mineral physics and geodynamics, the situation is different. We fully understand the theory of wave propagation, the behaviour of materials at high temperature and pressure, mass balance, momentum and energy equations. We can therefore generate training sets that will contain the complete physics of the corresponding problems.

Neural network were originally developed to mimic the behaviour of human brains. It is now clear that neural networks have little in common with biological neurons, but they remain very popular as pattern classifiers. The basic structure is a series of nodes that are joined by weighted non-linear functions. The nodes are organised in input-, output- and hidden layers (e.g. figure 44.1 in Mackay, 2003). The role of the training is to establish the weights that multiply the non-linear functions that constitute the nodes. The input layer contains the same number of nodes as there are data points. The number of nodes in the output layer is equal to that of the number of parameters chosen to describe the model. Usually one hidden layer is sufficient to model arbitrary complex functions (Bishop, 1995) and there are rules for choosing the number of nodes for the hidden layer. The weights are found by a robust non-linear optimization, know as back-projection (Bishop, 1995; Mackay, 2003). Such a neural network can be set up to solve the data assimilation problem where the inputs are the geophysical and geochemical observables and the outputs are the parameters entering the flow calculations.

While it is in itself interesting to obtain these input parameters for Earth-like thermo-chemical convection, it is equally important to know how well these parameters are constrained. This can be achieved by requiring the outputs to be in the form of probability density functions (pdfs). We successfully trained neural networks which produced pdfs for the depth on major discontinuities, elastic parameters and density using local phase velocities as input (Meier et al., 2007, 2009). Probability density functions are obtained by using mixture density networks (Bishop, 1995). We showed that these pdfs are equivalent to those obtained by Monte Carlo sampling. Neural networks and Monte Carlo techniques have complementary properties. While Monte Carlo techniques provide an answer to all model parameters simultaneously, neural networks only robustly infer one model parameter at a time. This is not a problem since the training of a neural network is very fast using the stable back-projection method. The obtained probability density can be seen as a marginal because the training set contains of course all the cases with all possible variations of the parameters. The interesting characteristic of neural networks is that they do not suffer from the curse of dimensionality (Meier et al., 2007). This means that far less model realisations are needed to train a successful network than would be needed in a classical Monte Carlo approach.

As mentioned above, a neural network is best trained on a single output pdf. Its maximum can be seen as the most likely value for that parameter and its width as a measure of how well this particular parameter is determined by the given observables. In the course of this project, we will extensively experiment to see which observables constrain a given parameter best. It is my experience that a simple input layer, one hidden layer, and a mixture density output layer is an appropriate network architecture. We will of course check if more complicated networks are required. I request a PhD student and more experienced postdoc based in Utrecht. They will join a group of 2 PhD students and 1 postdoc (see http://www.geo.uu.nl/~jeannot) working on more complicated neural network architectures (auto-encoders, convolutional and recurrent) for time domain waveform inversion.

The PhD student will design and train networks associating power spectra of seismic models to various convection parameters (Rayleigh number, viscosity law, chemical density contrasts, fraction of primitive material, Clapeyron slopes of phase transitions, concentrations of trace elements, …). Deschamps et al. (2007) found that power spectra are most informative to discriminate between thermo-chemical flow models. Many flow models need to be generated quickly to build a training set. A 2-D (much faster) version of StagYY in a spherical annulus will therefore be used. Hernlund and Tackley (2008) showed that the spectra obtained with the spherical annulus calculation match those of the full 3-D calculations. Therefore these simulations are appropriate to test the data sensitivity to a given parameter and the network architecture. At the beginning stages of the work, the student will spend some time at ETH to learn how to use the existing convection codes. The flow calculations will generate fields for temperature and chemical distributions, which will be converted into seismic wave speed and density variations using the software package Perple_X (Connolly, 2009; http://www.perplex.ethz.ch) where the latest mineral physics data and the self-consistent equation-of-state of Stixrude and Litghow-Bertelloni (2005, 2011) have been implemented. An important question is whether the chemical components are in thermodynamic equilibrium or exist as a simple solid mixture. We will test both scenarios and consider them as unknown parameters to be determined by the neural network as well. In a first stage, existing tomographic models will be used (e.g. Trampert et al., 2004), later the ones produced in the observational work package.

The postdoc will train neural networks on geochemical and geophysical observations, either individually to investigate data sensitivity or together. In the beginning, 2-D codes will be used, which are readily available (Xie and Tackley, 2004a,b). Input parameters will be varied in reasonable ranges (based on literature reviews) and He and Ar isotope ratio distributions and outgassing will be evaluated at different time steps.

These will be compared to geochemical observations found in data repositories (http://georoc.mpch-mainz.dwdg.de, http://www.petdb.org) and can therefore easily be used as input data for training a neural network. Geochemical data will first be used alone, but later also in combination with heat flow and gravity data and seismic models to investigate the improvement in parameter determination. At the start of the work, the postdoc will spend some time at ETH to learn how to manipulate the convection codes. In a similar way, the isotope system U-Th-Pb and Re-Os will be used, first alone and then in combination with geophysical observables. As mentioned in the challenges, tracking simultaneously noble gases and isotope system has not been done yet. This will be implemented in the geodynamics package and as soon as results become available, both types of geochemical observables will be used together.

- Supervisors: PI and Paul Tackley
- Support for one PhD student and one postdoc are requested for this part of the proposal
- Deliverables: iv
- Resources: Dedicated high-performance computer cluster requested by this proposal, existing 2-D convection software, know-how in neural network design
- Novelty: Using neural networks to infer input parameters for convection models from geophysical and geochemical data.

4 Synthesis

Geodynamic models in 3-D spherical geometry including all physical parameters and the tracking of geochemical data will start to become available from year 3. We will then start to build a database with time steps from models with varying all relevant parameters, which can reasonably be determined. The latter have been identified in the first years of the neural network package. We target an average 45 km resolution, which corresponds to about 7 million cells and about ten as many tracers to avoid artificial diffusion. Such a run will take about 1 week on 128 cores. On a 6144-core machine we will be able to produce 2496 models per year. To store one frame about 4Gb of disk space is required. We estimate to need a database of 5 frames per model and a run over 2 years will need about 100Tb of storage space. At the end of the project this database will be made available to the international community for benchmarking or other research projects. A neural network will be trained for each parameter using the same set of model simulations and input data. The latter is important to avoid biased parameter determinations and thus increase our confidence that these are indeed the most Earth-like parameters. Analysing flow models obtained with the most likely parameters will provide new information of the thermal and chemical evolution of our planet, for the first time providing models that are simultaneously consistent with the main different geophysical and geochemical datasets. The PI, Paul Tackley and the postdocs of the research group will do this work together.

- Deliverables: v and vi
- Resources: Dedicated high-performance computer cluster requested by this proposal
- Novelty: Thermo-chemical convection models in agreement with available geophysical and geochemical data will be produced.

We are fully aware that this is highly ambitious proposal, but at the same time we are confident of its success. Most tools are in place, and by using them in a systematic way, together with a dedicated high-performance computer, will allow the proposed research group to provide an integrated understanding of seismic tomography, gravity, heat flow, geochemical trace element data, mineral physics data and convection models and thus of Earth's thermo-chemical evolution over geologic times.

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d. Ethical and security-sensitive issues

ETHICS ISSUES TABLE

Areas Excluded From Funding Under FP7 ***(Art. 6)***

(i) Research activity aiming at human cloning for reproductive purposes;

(ii) Research activity intended to modify the genetic heritage of human beings which could make such changes heritable (Research relating to cancer treatment of the gonads can be financed);

(iii) Research activities intended to create human embryos solely for the purpose of research or for the purpose of stem cell procurement, including by means of somatic cell nuclear transfer;

All FP7 funded research shall comply with the relevant national, EU and international ethics-related rules and professional codes of conduct. Where necessary, the beneficiary(ies) shall provide the responsible Commission services with a written confirmation that it has received (a) favourable opinion(s) of the relevant ethics committee(s) and, if applicable, the regulatory approval(s) of the competent national or local authority(ies) in the country in which the research is to be carried out, before beginning any Commission approved research requiring such opinions or approvals. The copy of the official approval from the relevant national or local ethics committees must also be provided to the responsible Commission services.

	Research on Human Embryo/ Foetus	YES	Page
	Does the proposed research involve human Embryos?		
	Does the proposed research involve human Foetal Tissues/ Cells?		
	Does the proposed research involve human Embryonic Stem Cells (hESCs)?		
	Does the proposed research on human Embryonic Stem Cells involve cells in culture?		
	Does the proposed research on Human Embryonic Stem Cells involve the derivation of cells from Embryos?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

	Research on Humans	YES	Page
	Does the proposed research involve children?		
	Does the proposed research involve patients?		
	Does the proposed research involve persons not able to give consent?		
	Does the proposed research involve adult healthy volunteers?		
	Does the proposed research involve Human genetic material?		
	Does the proposed research involve Human biological samples?		
	Does the proposed research involve Human data collection?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

	Privacy	**YES**	**Page**
	Does the proposed research involve processing of genetic information or personal data (e.g. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?		
	Does the proposed research involve tracking the location or observation of people?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

	Research on Animals[2]	**YES**	**Page**
	Does the proposed research involve research on animals?		
	Are those animals transgenic small laboratory animals?		
	Are those animals transgenic farm animals?		
	Are those animals non-human primates?		
	Are those animals cloned farm animals?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

	Research Involving non-EU Countries (ICPC Countries[3]**)** [4]	**YES**	**Page**
	Is the proposed research (or parts of it) going to take place in one or more of the ICPC Countries?		
	Is any material used in the research (e.g. personal data, animal and/or human tissue samples, genetic material, live animals, etc) : a) Collected in any of the ICPC countries?		
	b) Exported to any other country (including ICPC and EU Member States)?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

	Dual Use	**YES**	**Page**
	Research having direct military use		
	Research having the potential for terrorist abuse		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	YES	

If any of the above issues apply to your proposal, you are required to complete and upload the "B2_Ethical Issues Annex" (template provided).

Without this Annex, your application cannot be properly evaluated and even if successful the granting process will not proceed.
Please see the Guide for Applicants for the Advanced Grant 2012 Call for further details and CORDIS http://cordis.europa.eu/fp7/ethics_en.html for further information on how to deal with Ethical Issues in your proposal.

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[2] The type of animals involved in the research that fall under the scope of the Commission's Ethical Scrutiny procedures are defined in the Council Directive 86/609/EEC of 24 November 1986 on the approximation of laws, regulations and administrative provisions of the Member States regarding the protection of animals used for experimental and other scientific purposes Official Journal L 358 , 18/12/1986 p. 0001 - 0028

[3] In accordance with Article 12(1) of the Rules for Participation in FP7, 'International Cooperation Partner Country (ICPC) means a third country which the Commission classifies as a low-income (L), lower-middle-income (LM) or upper-middle-income (UM) country. Countries associated to the Seventh EC Framework Programme do not qualify as ICP Countries and therefore do not appear in this list.

[4] A guidance note on how to deal with ethical issues arising out of the involvement of non-EU countries is available at: ftp://ftp.cordis.europa.eu/pub/fp7/docs/developing-countries_en.pdf