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Geodynamic Mantle Modeling and its Relation to Origin and Preservation of Life

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Summary. Section 1 refers to hypotheses on the origin of life. These different hypotheses require distinct geodynamic and structural-geology prerequisites. E.g., in case of chemoautotrophic metabolism-first hypotheses, a plate-tectonic mechanism is necessary that contains sites of reducing volcanic exhalations. It was shown that the mass extinctions of biological species are influenced by the convection-differentiation mechanism of the endogenic evolution of the Earth's mantle. Especially LIP-producing eruptions appear to be the principal reason for mass extinction events. Occasionally, bolide impacts cause an extinction event in an ecologically stressed, LIP-generated situation. Section 2 reports on our efforts pertaining to the self-consistent modeling of plate tectonics. To facilitate plate-like motions, two conditions are required, namely a low-viscosity asthenosphere and a deviation from the purely viscous constitutive equation of the lithosphere. Our modeling results show that already relatively simple additional assumptions in a 3-D spherical-shell model of the Earth's mantle produce oceanic lithospheric plates moving along the Earth's surface and changing their shape and size as a function of time. Section 3 describes a new model of episodic growth of continental crust (CC). In the case of genetics-first hypotheses or of metabolism-first hypotheses with solar irradiation or lightning energy supply, the existence of CC with epicontinental seas, lagoons and ponds is directly determining for the origin of life. Furthermore, the most important sources of nutrients originate from the upper CC. We put a water-concentration dependent solidus model of mantle peridotite into a 3-D spherical-shell, dynamic mantle model with chemical differentiation that redistributes the heat-producing elements. As a result, we obtain a set of temporal distributions of CC growth episodes that show a certain temporal invariance for a variation of the melting-criterion parameter, f_3. The laterally averaged surface heat flow density qob, the Urey number Ur, and the kinetic creep energy E_{kin} show temporally sinusoidal components superposing a monotonously decreasing curve. Section 4 discusses partly unknown distributions of physical quantities, the knowledge of which is necessary for the computation of a dynamic Martian convection-differentiation system. It is ambiguous whether the early strong Martian magnetic dipole was generated by the more effective core cooling due to a plate-tectonic mode of solid-state convection in the Martian mantle during the first 500 Ma. Section 5 outlines the numerical progress in the advancement of

the Terra code that was achieved by cooperation of the international group of Terra developers.

1 What has life to do with the endogenic dynamics of Earth and Mars?

1.1 Introduction: Definition of Life

It is difficult to define life and the biological species more precisely. *Barbieri* [5] specified life as follows. Life is a metabolizing material informational system with the ability of self-reproduction with changes (evolution), that requires energy and suitable environment. *Trifonov* [122] investigated 123 definitions of life and found a "lowest common denominator" as follows: Life is self-reproduction with variations. An overview of the problem is given by [45] . The definition by *Ruiz-Mirazo et al.* [100] is somewhat more specific: Living beings are autonomous systems with open-ended evolution capacities. They must have a semi-permeable active boundary, an energy transduction apparatus and, at least, two types of functionally interdependent macromolecular components. The latter is required to articulate a phenotype-genotype decoupling.

With regard to the species, the definition of *Mayr* [77] is customary: Species are groups of interbreeding natural populations which are reproductively isolated from other such groups. *Van Regenmortel* [124] objects that interspecies hybridization is quite common, especially in the plant kingdom and that many Archean and Proterozoic organisms did not reproduce by sexual means. Furthermore, we want to emphazise that biologists and paleontologists use differing definitions of the term species.

As it seems, reproduction is the most conspicuous feature of life. Animate beings carry their blueprint in the form of a genetic code which enables them to produce individuals that are *in principle* of the same type. Because living beings are objects of an extremely high degree of order and on account of the second law of thermodynamics, their existence is only possible by metabolism, i.e. they are materially and energetically open systems. A further consequence of the second law is the fact that at least all more complex living beings grow old and finally decease. A further complexity is hidden in the words *"in principle"*. Paleontologically, we observe a very slow, gradual alteration of the fossil's shapes whereas the extinction of a species is or seems to be abrupt.

1.2 Extinctions

In the Phanerozoic, i.e. in the last 570 Ma, we observe six large mass extinctions where up to 19 families of marine invertebrates and vertebrates died off during 1 Ma [94] . If, relating to extinctions, the word "large" is defined

Table 1. The five large Phanerocoic mass extinction events. Data acc. to [6], * after [105] .

Event	Final age (Ma)	Duration (Ma)	Loss of genera	Estimated loss of Species
Ordovician	443	3.3 to 1.9	57%	86%
Devonian	359	29 to 2	35%	75%
Permian	251	2.8 to 0.16	56%	96%
Triasic	200	8.3 to 0.6	47%	80%
Cretaceous	65	≤ 2.5	40% (60% *)	76%

by a loss of over 75% of estimated species then we determine five large mass extinction events during the Phanerozoic [6]. Cf. Table 1.

After every mass extinction, other families and species relatively quickly occupied the free living environment. At first sight, it looks like a discontinuity in the development of life.

What is the cause of the large mass extinction events? *The first explanation.* Independent of the present problem, it is evident that the terrestrial magnetic dipole and the magnetosphere serves as a protective shield for the genetic material. Therefore it is an essential prior condition for the continuity of life because the majority of the highly energetic, electrically charged particles of the solar wind and of the cosmic "radiation" are deflected. That is why it is understandable that one of the first proposals of an explanation of the mass extinction events was the assumption that the magnetic dipole reversals cause the mass extinctions. If we investigate the observations in detail we find, however, that, e.g., the large mass extinction at the Cretaceous-Paleocene Boundary (KPB) does *not* coincide with any magnetic dipole reversal. The temporal distribution of the Phanerozoic dipole reversals is now comprehensively known. It totally differs from the distribution of Phanerozoic mass extinctions. A magnetic dipole reversal takes only a period of 2000 to 5000 a. During this process, the magnetic dipole moment declines to 20 to 30 % of the original amount, however, the quadrupole and octupole contributions rise in this time span. Evidently, the magnetic protection of life is provided during these time intervals so that this first explanation fails.

The second explanation. Alvarez et al. [2] report on iridium increases of about 30, 160, and 20 times in deep-sea limestones exposed in Umbria, Denmark, and New Zealand. On the other hand, the upper continental crust is depleted in platinum metals. Because these iridium anomalies arose precisely at the time of KPB, *Alvarez et al.* [2] proposed that the impact of an asteroid had caused both the KPB mass extinction event and the iridium anomaly. *Schulte et al.* [105] confirm that the Cretaceous-Paleogene extinction coincided with the Chicxulub impact and that a global perturbation of the δ^{13}C curve and a drop of carbonate sedimentation in the marine realm simultaneously took place. However, they emphasize that these relatively sudden variations occured within the time of Deccan flood basalt volcanism but not at its beginning. They and also *Miller et al.* [82] conclude that the Chicxulub impact triggered the mass extinction. *Renne et al.* [95] show $^{40}Ar/^{39}Ar$ data and establish synchrony between KPB and the corresponding mass extinction to within 32 ka. However, they indicate that the global climate instability began with six abrupt temperature drops already $\sim$1 Ma *before* the Chicxulub impact [140].Therefore it is evident that the ecosystem was under critical stress already *before* the Chicxulub event. *Johnson and Hickey* [57] investigated the loss of flora around the KPB in North Dakota and showed that many species died off conspicuously *before* the KPB. Also the decrease of the number of Antarctic invertebrate species distinctly begins *before* the KPB [143]. *Benest and Froeschlé* [9] systematically compared the marine extinction events from the Lower Cretaceous until the present time with the age estimates of large impacts. They found a coincidence only for the KPB and for the Eocene-Oligocene Boundary but else not at all. In India, the dinosaurs and some fish and frog species died off somewhat *before* the KPB. Damage cannot appear before an impact if the impact is the only cause. On the other hand, there are also big impacts without any extinction event. Therefore, the suspicion raised that impacts only amplify the effect of another main mechanism.

The third explanation. Courtillot et al. [24] and *Archibald* [4] proposed that large eruptions of continental and oceanic flood basalts are the chief cause of mass extinction events. The giant volcanic eruptions not only produce the large igneous provinces (LIPs) [21] but also rise to a reduction of the solar irradiation into the atmosphere. The latter effect is caused by the volcanic change of the chemical composition of the atmosphere, particularly by aerosols and SO_2 gas emissions. Sulfur dioxide forms sulfate aerosol particles that reflect the incoming solar radiation [65]. Thereby a global cooling is caused [140] which effectuates a growth of the polar ice caps. Thus large areas of the epicontinental seas will become lowland. Already *Smith* [109] showed that the extinctions at the Triassic-Jurassic Boundary and at KPB are connected with worldwide regressions of epicontinental seas.

According to [19, 46, 64, 65] , studies of the Deccan Volcanic Province revealed three major volcanic phases: Phase-1 in C30n at 67.4 Ma followed by a 2 Ma period of quiescence, the main Phase-2 in C29r just before the KPB, and the late Phase-3 in the early Danian (C29r/C29n). Phase-2 generates $\sim$ 80% of the 3500 m thick Deccan lava pile. *Keller* [64] believes that the catastophic effects of the Chicxulub impact have been overestimated and that the KPB mass extinction is essentially caused the volcanic main Phase-2 of the Deccan lava and gas eruptions.

The end-Triassic extinction at 201.4 Ma is tied to a sharp negative spike in $\delta^{13}C$. *Whiteside et al.* [138] analysed the δ^{13}C of n-C_{25}-n-C_{31} n-alkanes and of wood. *Schoene et al.* [103] confirm this result. Furthermore, *Schoene et al.*[103] and *Deenen et al.*[30] found rapid sea-level fluctuations and a global cooling. They confirm that the Triassic-Jurassic Boundary and the end-Triassic mass extinction correlate with the onset of flood volcanism in the Central Atlantic Magmatic Province to $<$150 ka.

A majority of authors [38, 59] [and some of their quotations] link the Siberian flood basalts through production of large amounts of sulfur with the end-Permian mass extinction. *Shen et al.* [107] report that U-Pb dating reveals an end-Permian extinction peak at 252.28 ± 0.08 Ma and that the negative δ^{13}C excursion lasted $\leq$ 20 000 a. Admittedly, they [107] concluded that a massive release of thermogenic CO_2 and CH_4 is a plausible explanation for this sudden collapse of the marine and terrestrial ecosystems. Also in this case, the flood basalt eruption is the proper cause.

The 260 Ma-old Emeishan volcanism in Southwest China and interbedded Middle Permian carbonates contain a record of the Guadalupian mass extinction connected with the extinction of 56 % of plant species in the North China Block [14, 139]. This extinction predates a major negative δ^{13}C excursion. There is a clear temporal link that suggests that the flood basalt eruptions triggered the Guadalupian extinction [14, 139].

LIPs are obviously considered a relevant cause for mass extinctions and justifiably so. It is disputed yet, what thereby evoked additional mechanisms could amplify the direct effect, e.g. a haline euxinic acidic thermal transgression [66]. There are indications that occasionally bolide impacts can destabilize an already strained state. Apart from that, bolide impacts often do not have any essential influence on the variation of the number of species. Independent of the extinctions, we observe that the longer lasting major orogenic intervals are connected with the main glaciations which effect life otherwise.

Apparently, mutation and recombination of genes always act on the populations. They produce a very slow alteration of a species: Related populations in successive layers often show moving changes, especially the microfossils. However, the connection of orders, families and genera is often obscure [37]. Evidently, extinctions clear the way for the resettlement of living environments which formerly were dominated by the extinct species. It is increasingly obvious that *the mass extinctions of biological species are influenced by the endogene evolution of the Earth's mantle, especially by LIP-producing eruptions.*

1.3 Origin of Life

In the strict sense we know neither how nor where life came into existence [15]. The genetic information is stored by the DNA (desoxyribonucleic acid) which will be transcoded into RNA (ribonucleic acid) and then translated into proteins [36]. In reference to life, we want to limit ourselves to the well-known DNA-RNA-protein triad and exclude transeunt speculations. The origin of life divides into two stages. The first stage gives rise to first replicable molecules, probably to RNA [29]. Amino acids, sugars, and other molecules of life can be generated in the laboratory. There are several suggestions where these prebiotic reactions could take place in the Archean. The second stage is how organic molecules form a protocell, i.e. a system with proteins, nucleic acids, and cell membranes. This second stage contains the unresolved root of the matter. The two stages are connected by the question, what originated first, DNA or proteins? Genetics-first hypotheses are widely spread and connected with the opinion that the synthesis of RNA nucleotides and oligonucleotides is fundamental (*Orgel* [90–92]). As precursors of RNA, several alternatives to RNA have been proposed, namely peptide nucleic acid (PNA) and threose nucleic acid. Possibly RNA was directly synthesized. This process could have facilitated by a catalytic system on the surface of minerals [92]. *Johnston et al.* [58] found ribozymes which are able to produce complementary copies of RNA molecules.

As a metabolism-first hypothesis we mention the papers by *de Duve* [26–28]. He proposes a protometabolism in a thioester world and supposes catalysis on multimers which stem from thioesters. It is a question of a sophisticated chain of reactions based on thioesters and Fe-S compounds which result in a complete protometabolism using energy supply by lightnings or ultraviolet (UV) irradiation. Already *Miller and Urey* [83] experimentally showed that aldehydes and amino acids are produced in an anoxic atmosphere of H_2O, CH_4, NH_3, H_2, CO_2, CO and N_2 by electrical sparks (lightnings). These experiments depend on external energy sources. For this configuration, Archean "warm little ponds" and lightnings on continental sites have been proposed.

A second metabolism-first hypothesis has been suggested by *Wächtershäuser* [126–129]. He assumes that chemoautotrophic microorganisms played the most ancient role in the biosphere. Therefore he proposes a chemoautotrophic origin of life in a volcanic iron-sulphur world. In this case, the energy has not an indirectly solar origin but is released at the mouths of churning deep-sea vents, e.g. at the black smokers which are bound to the Earth-embracing system of plate boundaries of the oceanic lithospheric plates. So, in the case of the Wächtershäuser hypothesis, the existence of oceans and plate tectonics is necessary for the emergence of life on Earth and perhaps also on Mars if there were an ocean and plate tectonics in the first about 500 Ma. In spite of the lower luminocity of the early Sun and the larger distance of Mars from the Sun, the early Mars had a *fluid* ocean because of an atmosphere of higher density [31, 39–41]. An important framework requirement for life is fluid water. Because of the lower atmospheric pressure, this temperature window for *present-day* Mars is between 273 K and 283 K. The inorganic nutrients of life are molecules such as H_2, N_2, H_2O, H_2S, NH_3, CH_4, CO, CO_2, HCN and P_4O_{10} [129]. These molecules emerge as volcanic exhalations from the planet's mantle. (O_2 and O_3 are considered to be virtually absent.) The listed multitude of molecules catalytically reacted at the electrically positively charged surfaces of metallic sulfides, e.g. FeS, NiS, ZnS, (Fe,Ni)S. Generelly expressed, transition metal centers with sulphido, carbonyl and other ligands were catalytically active and promoted the growth of organic superstructures [129]. *Wächtershäuser* [129] believes to be able to explain also the cellularization and the emergence of the genetic machinery. He also delineates the track from chemoautotrophic life to Bacteria, Archea and Eukarya. *Kundell* [70] demonstrated by computational analysis what special proto-nucleic acid could come into consideration as a pioneer organism.

Both genetics-first hypotheses and metabolism-first hypotheses encounter difficulties. *Vasas et al.* [125] indicate that, in case of metabolism-first hypotheses, replication of compositional information is so inaccurate that fitter compositional genomes cannot be maintained by selection and, therefore, the system lacks evolvability which, however, is an essential feature of life.

In case of genetics-first hypotheses and of metabolism-first hypotheses with solar UV radiation or lightnings as an energy source, the following geological conditions have to be fulfilled: It is imperative that there are continents with shallow epicontinental seas. Furthermore shallow and nearly or totally closed small lagoons or ponds with a primordial soup of organic compounds are preconditions. *In case of chemoautotrophic metabolism-first hypotheses, in addition to continents, a plate-tectonic mechanism is necessary which exhibits sites of reducing volcanic exhalations.* In this case solar energy is irrelevant, but only in the early stages. For all types of origin-of-life hypotheses, sources of nutrients are necessary. *Only three rock types serve as a source of nutrient [76], namely (a) tonalite-trondhjemite-granodiorite (TTG) complexes of the Archean upper continental crust (UCC), (b) carbonatite magmatic rocks enriched in U and Th, and (c) primordial continents with KREEP basalts which are rich in potassium (K), rare earth elements (REE) and phosphorus (P).* The last one is essential for life because it is a component of DNA, RNA and phospholipids that form the cell membranes.

1.4 Preservation of Life

The preservation of life depends on many geochemical conditions. The cycles of water, carbon, sulfur and phosphorus are very important. It makes sense to include the endogenous parts of these cycles which include the silicate mantles of Earth and Mars. The endogeneous water cycle has a bearing on both the effective shear viscosity and thus on mantle solid-state convection [104] and on the location- and time-dependent solidus and thus on chemical differentiation of the mantle [131]. Phosphorus has a restrictive effect on the biological productivity of the Earth [42]. In Subsection 1.2, we describe how geodynamics influences the large mass extinction events and the preservation of life. On the other hand, the products of life's metabolic processes have a profound effect on the chemistry of the Earth which possibly affects the mechanics of tectonic and magmatic evolution of the mantle [108]. As a survey on the specific problems of the chemistry of the Earth, we recommend [18], for the chemistry of Mars [33, 79, 88, 121].

The existence of an ocean is a necessary but not sufficient condition for plate tectonics which, in turn, is the most effective mechanism for a stronger cooling of the planet's iron core. If the core's ferrous alloy is not or not completely frozen then a sufficiently large cooling of the planet drives the hydromagnetic convection of the fluid part of the core. From the geomagnetic secular variation, it has been concluded that the magnitudes of the flow velocities in the metallic fluid of the Earth's outer core (OC) amount to 10 and 30 km/a. So the OC viscosity is between 1 and 100 Pa·s. Therefore, rather small eddies are expected which are oriented along the Earth's axis of rotation by the Coriolis force. The mechanism can be explained by the theory of averaged fields. The terrestrial magnetic induction field determines the magnetosphere which is the essential protection system of life. *Therefore plate tectonics is twofold or threefold important for life, first by the volatile cycles of the mantle, second by the magnetosphere and third by the black smokers if Wächtershäuser [129] is right. In the case of genetics-first hypotheses or of metabolism-first hypotheses with solar irradiation or lightning energy supply, the existence of continents with epicontinental seas, lagoons and ponds are directly determining for the origin of life. Because of the sources of nutrients, the origin and growth of the continental crust (CC) is relevant for life, in either case [76, 131].*

2 Self-Consistent Modeling of Plate Tectonics

It was a brilliant performance to recognize that a multitude of geological, kinematic, geochemical, isotopic and geophysical observations can be systematized by plate tectonics. But this systematization does not mean physical comprehension. Therefore, some pioneering papers derive the plate movements by self-consistent numerical modeling (*Trompert and Hansen* [123], *Tackley [116, 117]*, *Richards et al.* [96], *Bercovici and Karato* [11], *Bercovici and Ricard* [12]). This means that the plates are not artificially prescribed at the upper boundary of the model but they develop from the system of equations of mantle convection. In the following, we concentrate on our own papers because this is a statement of accounts on our use of supercomputing facilities at SCC Karlsruhe and HLRS Stuttgart.

We converted the balance equations of momentum, energy, and mass for our purpose [132]. E.g., the energy conservation was rewritten in such a way that the Grüneisen parameter, γ, explicitely occurs several times (cf. Eqns. (33), (34), (38) of [132] and (6) of [130]). Using the Vashchenko-Zubarev equation [55], we determine γ directly from seismic observations, i.e. from the Preliminary Reference Earth Model (PREM, [35]). In this way, it is not necessary to use mineralogical mantle models to determine γ. To estimate the buoyancy, we need the gravity, g, and the thermal expansivity, α, as a function of radius, r. We use the parameterized form of gravity from PREM. As for the expansivity, we adopt a modified version of the model by *Chopelas and Boehler* [20]. Using

$$\gamma_{th} = \frac{\alpha \cdot K_T}{c_v \cdot \rho} = \frac{\alpha \cdot K_S}{c_p \cdot \rho} \tag{1}$$

taking the adiabatic bulk modulus, K_S, and the density, ρ, from PREM, α from [20], and equating the thermodynamic Grüneisen parameter, γ_{th}, with the Vashchenko-Zubarev gamma, we are able to determine c_p, the specific heat at constant pressure.

The temperature and pressure dependence of the shear viscosity, η, is, however, a good deal more critical for the solution of the balance equations. Both the *energy balance*

$$\frac{\partial T}{\partial t} = -\frac{\partial (T v_j)}{\partial x_j} - (\gamma - 1) T \frac{\partial v_j}{\partial x_j} + \frac{1}{\rho c_v}\left[\tau_{ik}\frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j}\left(k \frac{\partial}{\partial x_j} T\right) + \mathcal{Q}\right] \quad (2)$$

and the *momentum balance*

$$0 = -\frac{\partial}{\partial x_i}(P - P_r) + (\rho - \rho_r) g_i(r) + \frac{\partial}{\partial x_k}\tau_{ik} \quad (3)$$

include the deviatoric stress tensor, τ_{ik}, where

$$\tau_{ik} = \eta\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3}\frac{\partial v_j}{\partial x_j}\delta_{ik}\right) \quad (4)$$

and the viscosity, η,

$$\eta = \eta(r, \theta, \phi, t) = 10^{r_n} \cdot \frac{\exp(c\, \overline{T_m/T_{av}})}{\exp(c\, \overline{T_m/T_{st}})} \cdot \eta_3(r) \cdot \cdot \exp\left[c_t \cdot T_m \left(\frac{1}{T} - \frac{1}{T_{av}}\right)\right] \quad (5)$$

K_T is the isothermal bulk modulus, c_v specific heat at constant volume, T temperature, t time, x_j position vector, v_j velocity vector of solid-state creeping, k thermal conductivity, $\mathcal{Q}$ heat generation rate per unit volume, P pressure, g_i gravity vector, θ colatitude, ϕ longitude, r_n viscosity-level parameter, c_t and c=7 are parameters (see [130]), T_m melting temperature, T_{av} laterally averaged temperature, T_{st} starting temperature, η_3 radial viscosity profile (see [130]), the indices r at P_r and ρ_r refer to the adiabatic reference state.

From the postglacial uplift of continents, e.g. Fennoscandia and Laurentia, it is evident that the asthenospheric viscosity is 10^{21} Pa·s. Therefore and on account of the profile η_3, we choose η_3=3.45·10^{20} Pa·s at 367 km depth [130]. Geophysical multi-layer models often assume a certain number of layers where every layer has a constant viscosity. *Sabadini and Vermeersen* [101] give an excellent survey of applications of normal mode relaxation theory to the derivation of terrestrial viscosity profiles. We [133] introduced a new viscosity profile of the Earth's mantle and supplemented [135] it to introduce a numerically feasible approach to take account of the mantle's secular cooling and the slow rising of the viscosity profile using the second factor on the right-hand side of Eq. (5). Some ideas of [135] are listed as follows.

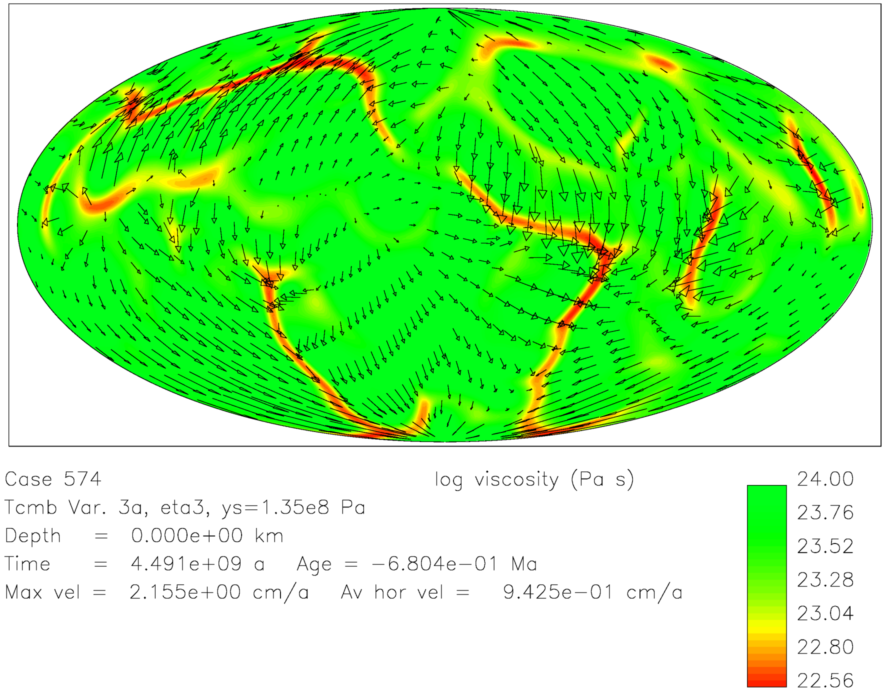

Fig. 1. Modeling of self-consistent oceanic lithospheric plates in a 3-D dynamic spherical shell according to [133]. This equal-area projection shows a log-viscosity (Pa· s) distribution with a yield stress of 135 MPa in the lithosphere. This solution type was obtained in a larger Ra-σ_y area by parameter variation. Ra denotes the Rayleigh number. Arrows show the plate-like array of creeping velocities of the lithospheric rocks.

(a) A chemically homogeneous layer of the mantle cannot have a constant viscosity because of the pressure dependence of activation enthalpy. Therefore, the viscosity mostly rises with pressure. A compensation or even overcompensation by the temperature dependence is virtually possible only near the core-mantle boundary (CMB) because of the extremely high temperature gradient in the D" layer.

(b) Viscosity discontinuities occur in the chemically homogeneous parts of the mantle only at phase boundaries, because P and T do not jump.

(c) At 410, 520 and 660 km depth, the lattice of olivine changes toward denser packings of atoms. Therefore it would be inconsistent to assume that there only the seismic velocities, v_s and v_p, and the density, ρ, jump but not activation energy and activation volume. Because the activation enthalpy is in the exponent of the viscosity function, we expect appreciable viscosity jumps.

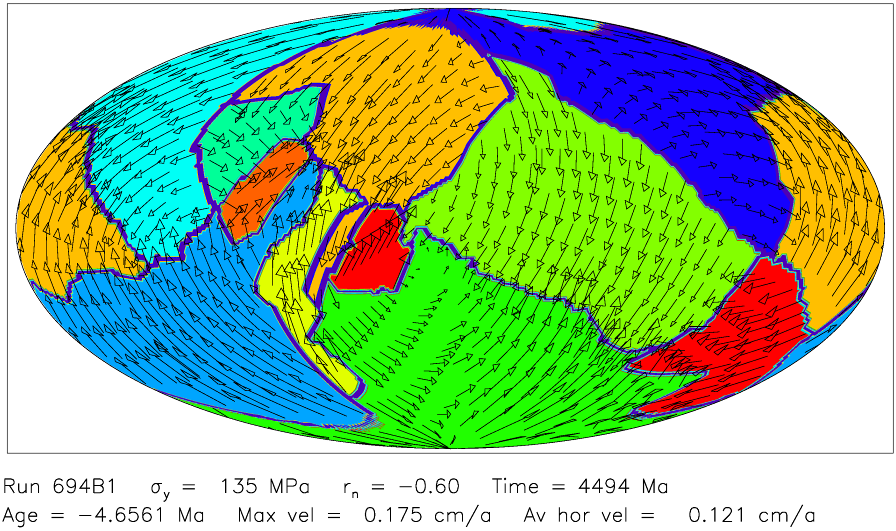

Fig. 2. Improved lithospheric plates (colors) and creep velocities (arrows) for a 3-D convection model [130] with chemical differentiation and continents which are not shown here. For decreasing r_n, the viscosity difference between oceanic lithosphere and asthenosphere grows and the number of lithospheric plates decreases if the other parameters are fixed.

Therefore we had considerable numerical problems with the Terra code and encouraged corresponding efforts (*Müller* [87], *Köstler* [69]).

(d) Other authors often use only the temperature dependence of viscosity to numerically produce an ocean lithosphere. But the real ocean lithosphere evolves not only from the temperature dependence but also by dehydration, other devolatilizations and not least by chemical differentiation. The latter one generates a basaltic and gabbroic ocean crust, underneath a harzburgitic layer and under it a lherzolithic layer. Therefore the lithosphere-asthenosphere boundary (LAB) corresponds to a *chemical* jump and a viscous jump. That is why we introduced a stiff lithosphere in our viscosity profile, $\eta_3(r)$. For numerical reasons, however, we had to replace the η-jump by a steep viscosity gradient. It can be shown by numerical experiments that *it is not possible to obtain self-consistent plates near the surface of a spherical shell if we use a purely viscous constitutive equation.* Therefore we additionally introduced a viscoplastic yield stress, σ_y. For the uppermost 285 km, an effective viscosity, η_{eff}, was implemented where

$$\eta_{eff} = \min\left[\eta(P,T), \frac{\sigma_y}{2\dot{\varepsilon}}\right], \tag{6}$$

The second invariant of the strain rate tensor is denoted by $\dot{\varepsilon}$. *The second essential condition for the appearance of self-consistent plates is the low-*

viscosity asthenosphere in η_3. Using these principles we [133] calculated Fig. 1. Further developments of the model are demonstrated in [130]. Fig. 2 shows an improved plate-like behavior.

3 Modeling of Continental Growth

The formation of basaltic oceanic crust occurs by a single-stage melting of the depleted mantle (DM) near mid-ocean ridges (MOR). According to [53], 30 to 80% of the Earth's mantle are depleted (DM) in incompatible elements (e.g. U, Th, K, REE), according to [10], 30 to 60%. The low-viscosity asthenosphere is preferably composed of DM. This fact is verified by observations at MOR. However, the production of continental crust (CC) is considerably more complex. Furthermore, the chemical composition of the lower continental crust (LCC) is not accurately known [98]. It is assumedly andesitic or at the boundary between andesite and basaltic andesite, i.e. at about 56.5 wt % SiO_2 [118–120]. A minimum of two stages of chemical differentiation are necessary to produce granodiorite-dominated upper continental crust (UCC) [118]. *Davidson and Arculus* [25] present five conceptional models for generating CC where particularly Model V appears to be realistic. According to the last model, CC essentially evolves from oceanic island arc crust (OIAC). For instance, the crustal structure of the Izu-Bonin island arc [115] may be considered as a prototype of OIAC. After the orogenic shortening, an ultramafic cumulate resides beneath the seismological Moho. This cumulate ranges down to the genetic Moho. After continuing orogenic thickening, this cumulate and the subjacent lithospheric mantle will be removed by thermal erosion through convection in the space of sub-arc wedge or by delamination through a Rayleigh-Taylor instability. A presumably somewhat smaller part of the CC-growth emerges from the accretion of oceanic plateau basalts which result from increased plume activity. Meanwhile we have got evidence that the juvenile plateau basalt proportion of the total basalt production of an orogenically active period was considerably larger than that of the present time. Furthermore, these orogenic events took place episodically [21]. We [131] did not include the specific CC-differentiation with full details into our global convection model but in a simplified way. We designed a new dynamic 3-D spherical-shell convection model of the Earth's mantle and incorporated a novel solidus, T_{sol}, [72] of peridotite which is not only a function of pressure, P, but also of water concentration. Partial melting in major volumes occurs only when

$$T > f_3 \cdot T_m \tag{7}$$

applies or when the total water abundance exceeds the water solubility [72, 81]. The quantity f_3 is a parameter that is somewhat smaller than or equal to 1 and that we vary in the different Terra runs. Because plenty of water escapes during every chemical differentiation event, the solidus will be enhanced for some time after the differentiation event in the differentiation volume. We use the concept of chemical mantle reservoirs considerably different than in previous times [52, 53]. We do not imagine sharp boundaries between the reservoirs but we define the time-dependent chemical composition of a specific mantle location by the mixing ratio of the conventional reservoirs using the reservoir concentrations of the incompatible elements by *McCulloch and Bennett* [78]. We use the three chemical mantle reservoirs (CC, DM, PM) with different abundances [131] of heat-producing elements U, Th, and K. The segregation processes quickly change the distribution of these elements; the solid-state mantle convection slowly modifies the distribution. Because the heat generation rate per unit volume, $\mathcal{Q}$, depends on the temporally and spatially variable U, Th and K abundances, there is a feedback on convection and thermal evolution of the mantle. Zircon and sandstone age estimates result in *observed* peaks of frequency at 2697, 1824, 1435, 1047, 594, 432, and 174 Ma. *These episodes are reproduced by run 498* (cf. Fig. 3, first panel). Our model [131] is based on the numerical solution of the balance equations of energy, momentum, moment of momentum, and mass in a spherical shell which represents the Earth's mantle. Furthermore, we use equations which guarantee the conservation of the four sums of number of atoms of the pairs ^{238}U-^{206}Pb, ^{235}U-^{207}Pb, ^{232}Th-^{208}Pb, and ^{40}K-^{40}Ar. In the present model of continental evolution, we replaced the viscosity profile $\eta_3(r)$ [130, 133] of Eq. (5) by the newly developed $\eta_4(r)$ [131] which resembles the viscosity profile by *Mitrovica and Forte* [84] although the derivation of it was completely different. The radial dependence of viscosity, $\eta_4(r)$, is based on some solid-state physics considerations. We took the mean of the relative viscosity between LAB and a depth, h, of 1250 km. The absolute value of this mean was defined as 10^{21}Pa·s, i.e. the observed Haskell value. Furthermore, the Grüneisen parameter, γ, is important for solid-state geophysics [3, 60, 93, 113, 114]. Cf. Eq. (2) and the Gilvarry-Lindemann equation [134], Eq. (2.8). In [130, 133], we utilized the Vashchenko-Zubarev gamma, γ_{VZ}. Because, however, the shear modes contribute an essential part to γ, we [131] replace γ_{VZ} by the acoustic gamma, γ_a, where

$$\gamma_a = \frac{1}{6}\frac{K_T}{K_S + (4/3)\mu}\left[\left(\frac{\partial K_S}{\partial P}\right)_T + \frac{4}{3}\left(\frac{\partial \mu}{\partial P}\right)_T\right] + \frac{1}{3}\frac{K_T}{\mu}\left(\frac{\partial \mu}{\partial P}\right)_T - \frac{1}{6} \tag{8}$$

The quantity K_S denotes the adiabatic bulk modulus and μ the shear modulus. For the depth interval between 771 and 2741 km, we [131] use the observed seismic PREM values and Eq. (8) to determine γ_a. For $h <$771 km and in the thin D" layer immediately above the CMB, the observed dK/dP and $d\mu/dP$ of PREM lead to physically implausible depth variations of γ. Therefore, we employ the gamma estimates of [113] for the latter depth ranges. The combined Grüneisen parameter is called extended acoustic gamma, γ_{ax},

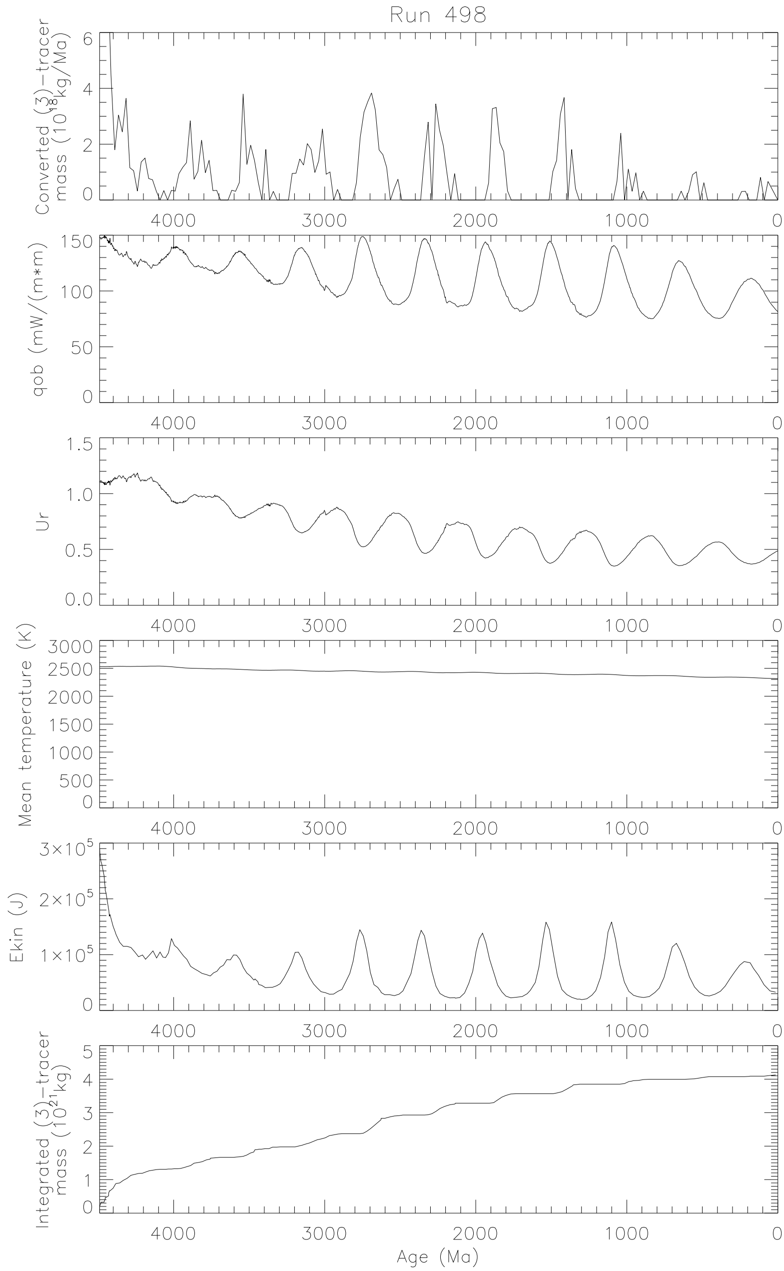

Fig. 3. Evolution curves of run 489. This case was found by variation of four parameters [131], namely, Rayleigh number, Ra, viscoplastic yield stress, σ_y, thermal conductivity, k, and melting-criterion parameter,f_3. For this run, the viscosity-level parameter is r_n=0.5 (This equates to about Ra=10^8), σ_y=120 MPa, k=5.0 W/(m·K), and f_3=0.995. The first panel shows the episodic, juvenile CC-magmatic activity, the second one the laterally averaged surface heat flow density, qob, and the third one the Urey number, Ur. The fourth panel displays the volumetrically averaged mantle temperature, T_{mean}, the fifth one the kinetic energy, E_{kin}, of the solid-state convection of the mantle. The sixth panel, finally, represents the CC cumulative growth.

that finally has been used in [131]. Furthermore, we [131] derived improved profiles of $\alpha(r)$ and $c_v(r)$. Because we now adopt the water-abundance dependent solidus [72], our viscosity function [131] also depends on the water concentration (cf. Eq. (5)), in contrast to [130, 133]. As a result, there are magmatically quiescent time intervals between the active periods (Fig. 3, first panel). Furthermore, qob (Fig. 3, second panel), Ur (Fig. 3, third panel), and E_{kin} (Fig. 3, fifth panel) distinctly show temporally sinusoidal components which are superimposed to slowly decreasing curves. However, the volumetrically averaged mantle temperature, T_{mean}, *does not change rapidly and is monotonously decreasing* (cf. Fig. 3, fourth panel). This result corroborates a principal conclusion of *Gurnis and Davies* [50]. Therefore, we can dismiss catastrophic mechanisms that *simultaneously* incorporate the *whole* mantle.

In our model, the number, size, form, distribution and angular velocity of the evolving continents is *not* prescribed or constrained. These quantities are a result of the dynamics of the numerical system. The only exception is the rule that if a terrane, e.g. an oceanic plateau, touches a continent, it has to be united with this continent. This regulation simulates the geological accretion of terranes. Fig. 4 shows a typical continental distribution for the geological present time. Of course, we can show the continental distribution also for earlier instants of time. To estimate whether we obtained a *realistic* solution, we developed the model continents of the modeled present time into spherical harmonics. Because the spherical-harmonics coefficients, A_n^m and

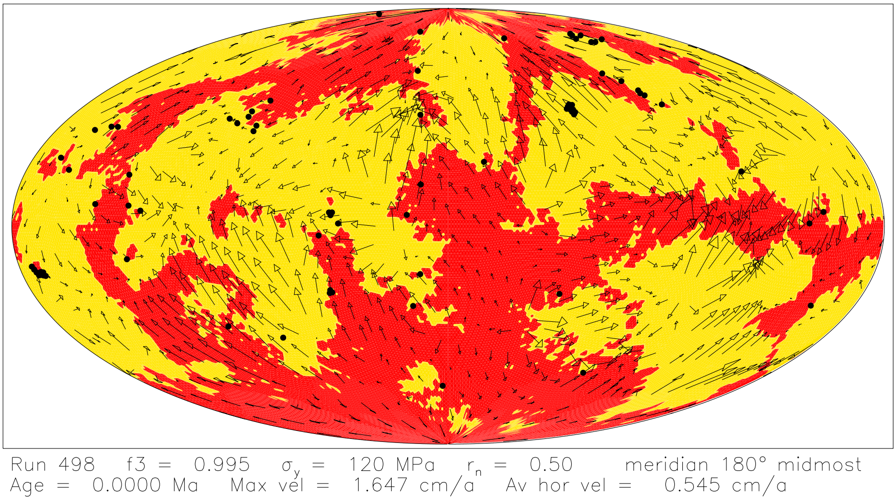

Fig. 4. Present-day distribution of continents (red), oceanic lithosphere (yellow) and oceanic plateaus (black dots) for run 498. The quantities r_n=0.5, σ_y=120 MPa, k=5.0 W/(m· K), and f_3=0.995 are kept constant. The arrows show the present-day creep velocities at the surface.

B_n^m, depend on the poles of the grid of parallels and meridians, i.e. on a human addition, we have to form pole-independent functions h_n of A_n^m and B_n^m. Then we compare the computed h_n with the h_n of the real, present-day distribution of continents. In this way, we found a realistic Ra-σ_y area. If we draw nearer to this special Ra-σ_y area in a wider Ra-σ_y space then also the other magnitudes, e.g. *qob*, converge to realistic values which are known from other investigations.

4 Considerations on a Numerical Model of the Thermal Evolution of Martian Mantle

Today it is clear that the Earth always had, exclusive of the earliest stages, fluid oceans, continents with sediment-producing running water and an atmosphere which initially was CO_2-rich and nearly anoxic. The animate beings themselves essentially contributed to the decrease of the CO_2 concentration in the terrestrial atmosphere by the sedimentation of limestone. This decrease diminished the greenhouse effect and balanced the luminocity increase of the sun. Therefore, the outlined mechanism works like a temperature control device. Hydrous mineral phases and the thereby produced diminished melting temperature in the upper layers of the Earth's oceanic lithosphere as well as the existence of an asthenosphere are essential preconditions for the mechanism of terrestrial plate tectonics. Plate tectonics, on the other hand, cools the Earth essentially more effective than a one-plate planet like the present-day Mars. This effective cooling, the *fluid* metallic core and a sufficiently large rotational speed are necessary for the sufficiently large magnetic dipole field of the Earth and the life-protective magnetosphere.

Is it possible to transfer this overall picture to the early Mars? On the northern Martian hemisphere, shore lines were found that point to an early ocean that covered about 42 % of the surface. It is notable that the Martian soils in the Meridiani Planum and in the Gusev Crater show a good correlation between the concentration of phosphates and those of sulphates and chlorides. The outcome of this is that a homogenization took place in a large water reservoir like an ocean [48]. Even if an early Martian ocean existed we cannot directly conclude that there was early plate tectonics.

Large empty fluviatile valleys have been observed on Mars. It is not clear, however, whether they represent previous rivers or streams due to episodic huge mud eruptions. At the Martian poles, water ice exists even in the present time. Numerous structures in mid-latitude regions of Mars point to previous glaciers with classical moraine structure. *Kargel* [61] supposes that the present-day Martian crust contains dikes of water ice, hydratized sulphates, clathrates etc. in a configuration similar to pegmatite dikes in the Earth's UCC. Also the shergottites, nakhlites, and Chassigny (SNC meteorites) are sign of a wet Martian mantle [79]. On the other hand, we cannot find any mid-ocean ridge system at the bottom of the ancient Martian ocean because it is covered with sediments. *Acuña et al.* [1] discovered that, in the first 500 Ma, Mars had a magnetic dynamo that disappeared before the Hellas and Argyre impacts that happened 4000 Ma ago. The intensity of the remanent field of the Martian crust is surprisingly high. Mars Global Surveyor revealed magnetic inductions $\geq$ 1500 nT in an altitude of 120 km. There are appreciable contributions to the Martian magnetic induction field for spherical harmonics degrees n $\geq$ 14 that are rather small on Earth. It is an unresolved problem whether the early Martian dynamo was particularly powerful or whether a quadrupolar dynamo is more probable [54, 71, 137]. ASPERA-3 results of Mars Express [74] suggest that the solar wind could cause the losing of ocean water and other volatiles. Therefore, the dynamo switching off would not only annihilate potential Martian life but also dry out the Martian ocean and heavily diminish the mass of Martian atmosphere.

In the strongly cratered highlands of the southern Martian hemisphere, there are intensive, EW striking anomalies of the radial and northern components of the magnetic induction field that have been associated with the terrestrial mid-ocean magnetic anomalies [22, 23, 112]. But the extent of these Martian anomalies is considerably larger. Furthermore, we would expect them at the bottom of the previous ocean on the northern hemisphere. Therefore, the problem of the Martian plate tectonics is unresolved.

Before we can design and compute a dynamic 3-D spherical-shell Mars model, we need a structural model analogous to PREM. This is a difficult task because Mars is virtually seismically not explored. Furthermore, the problem of the chemical model is not resolved. We know only the mass, moment of inertia, radius, tidal Love number k_2, the very well explored Martian surface and the SNC meteorites. But the SNCs are differentiation products that come from the crust and are *not* representative of the Martian mantle as a whole. *Sohl and Spohn* [111] derive two end-member structural models where they assume a bulk chondritic ratio Fe/Si=1.71 for the first model. For the second model, however, they hypothesize a maximum value $C = 0.366 * M_p r_p^2$ of the polar moment of inertia factor. They derive the density, ρ, and other physical parameters as a function of radius, r. Using a chondritic basic assumption, *Walzer et al.* [136] estimated ρ, the isothermal bulk modulus K_r, the thermal expansivity α, and the Grüneisen parameter γ as a function of depth of the Martian mantle. *Rivoldini et al.* [97] derive the density and other profiles for Mars where they use five different chemical bulk compositions as a presupposition, namely DW84 [33], LF97 [73], EH45 [102], EH70 [102] and MM03 [85]. The existing uncertainities of the Martian structural models are also illustrated by the fact that even up-to-date values of the tidal Love number range between 0.12 $\pm$ 0.004 [75] and 0.236 $\pm$ 0.058 [110] where a *probably* realistic value is at 0.159 $\pm$ 0.009 [68].

Modern *parameterized* convection models of Mars were presented by [16, 44, 51, 86, 106], where the model by [44] predicts that the Martian mantle must have been degassed more extensively (>80%) than previously thought. *Ogawa and Yanagisawa* [89] computed a *dynamical* 2-D Cartesian-box convection model of the Martian mantle. They present the evolution of temperature, internal heating, composition, and water content in 2-D boxes. The estimated plume magmatism is sufficiently strong to generate a large crustal growth and dehydration in the early Martian history. *Ruedas et al.* [99] give an account of another *dynamical* model, in this case in a 2-D spherical annulus geometry. To avoid the difficulties with the first 500 Ma of Martian history, only the thermochemical evolution of Martian mantle over the past 4 Ga was computed. The authors of [99] and [136] independently concluded that, of all the above named chemical Martian mantle models, the *Dreibus-Wänke* [33] model tends to explain observations best.

A future dynamic Mars model should solve the full set of balance equations of solid-state creeping in a 3-D spherical shell like the procedure for the Earth's mantle summarized in Sections 2 and 3. The first 500 Ma of Martian evolution should not be included. But for Mars, that involves some difficulties:

a) We have no seismic model corresponding to PREM. Therefore, we should derive a structural model analogous to *Sohl and Spohn* [111] or *Gudkova and Zharkov* [49]. Hence, a hypothetical seismic model and the radius dependence of some other physical quantities should be estimated using a chemical Martian mantle model. So, the most fundamental decision concerns the chemical model. *Dreibus and Wänke* [34] propose 40 % oxidized components of C1 carbonaceous chondritic material and 60 % heavily reduced material (component A). In contrast, *Sanloup et al.* [102] assume 45 % enstatite meteorites EH and 55 % ordinary chondrites of type H because they want to explain the isotope ratios of oxygen. However, they generate other difficulties with their proposal. Of course, every realistic structural model has to produce the correct values of the observed mass, moment of inertia, radius and tidal Love number, i.e. correct within the error limits. A further constraint is the conclusion, derived from satellite observations [142], that the CMB of Mars separates a solid upper domain from a liquid lower one. Since the Martian iron core is not frozen out, we have to look for another explanation of the missing present-day magnetic dipole field of major intensity.

b) The estimation of the effective shear viscosity of solid-state creep in the Martian mantle as a function of radius is yet considerably more difficult than for the Earth's mantle. In addition, we do not know a fixed point analogous to the Earth's Haskell value. Because of the formulas of Sections 2 and 3, it would be important to determine the temperature-pressure phase diagram of the Martian-mantle material. The resultant phase boundaries with jumps of activation energy and activation volume are relevant to determine the expected essential viscosity discontinuities. Furthermore, the pressure dependence of the solidus, T_{sol}, can be derived from the phase diagram. Moreover, there is a connection between the phase diagram and the Grüneisen parameter, γ, and the thermal expansivity, α. In the dynamic model, we need also the radius dependence of γ and α.

c) The structural model of a) cannot be derived independently of b) because the acoustic gamma, γ_a, depends on K, dK/dP, μ, $d\mu/dP$. Furthermore, the density, ρ, depends on K.

d) One could consider to adopt phase diagrams for a hydrous peridotite system [56, 62, 63] because the early Martian mantle probably had a higher water concentration than the Earth's mantle. But this is not so simple because the Earth's mantle contains a principal chemical component of about 8 % FeO whereas the Martian mantle probably contains 18 % FeO [13, 34].

e) We have to take into account that, also for Mars, the lithosphere does not simply develop in consequence of the temperature dependence of viscosity but also due to chemical differentiation and owing to the relation between water abundance and water solubility [81] as a function of depth.

f) We propose that the viscosity distributions of Earth [131] and Mars are also time-dependent because the water abundance is also temporally variable. If the early Martian mantle lost plenty of water then the curves of water solubility and water concentrations lose their two intersection points [81]. Therefore, the early Martian asthenosphere vanishes. But the asthenosphere is a prerequisite of plate tectonics.

g) Also the Martian lithosphere cannot resist shear stress in any order. Therefore, we should introduce a viscoplastic yield stress.

h) *The items a) to g) could possibly result in a model with early plate tectonics an Mars, early stronger core cooling and, consequently, a strong early Martian magnetosphere that was life-protective if life was existent.* In any case, we know that Mars had a strong magnetic dipole field in the first 500 Ma.

i) In contrast to Earth, the Martian mantle does not have a uniform $^{182}W/^{184}W$ ratio [43, 67, 80]. Therefore, Mars has a heterogeneous mantle [80]. That is why we expect that considerable deviations from the spherical-shell model are necessary.

j) Mars has only a basaltic crust, no felsic igneous rocks [80].

5 Numerical Improvements

We obtained the numerical solutions of the system of balance equations of convection in a spherical shell using a three-dimensional finite-element discretization, a fast multigrid solver and the second-order Runge-Kutta procedure. The mesh is generated by projection of a regular icosahedron onto a sphere to divide the spherical surface into twenty spherical triangles or ten spherical diamonds. A dyadic mesh refinement procedure connects the midpoints of each side of a triangle with a great circle such that each triangle is subdivided into four smaller triangles. Successive grid refinements generate an almost uniform triangular discretization of the spherical surface of the desired resolution. Corresponding mesh points of spherical surfaces at different depths are connected by radial lines. The radial distribution of the different spherical-surface networks is so that the volumes of the cells are nearly equal.

The details of the Terra code are given by *Baumgardner* [7, 8], *Bunge et al.* [17] and *Yang* [141] . For many runs that we needed for variation of parameters, we used a mesh with 1351746 nodes. Some runs were made with 10649730 nodes to check the convergence of the lower resolution runs. The result is that the laterally averaged surface heat flow, the Urey number, the Rayleigh number and the Nusselt number as functions of time show hardly any discernable differences (<0.5%). The code was benchmarked for constant-viscosity convection by *Bunge et al.* [17] with numerical results of *Glatzmeier* [47] for Nusselt numbers, peak temperatures, and peak velocities. A good agreement (≤1.5%) was found.

In 2009, an international group of Terra developers decided to set up a community svn-repository for further code development, supplemented by trac, a web-based project management and bug-tracking tool, and automated compile/test cycles using BuildBot. From then on the group worked on a common code base using automated tests for every revision of the code. The group enhanced the code to increase global resolution and maximum number of MPI processes. A Ruby test framework was integrated [87] into the automated BuildBot tests, and a finite-element inf-sup stabilization using pressure-polynomial projections [32] was implemented. An efficient preconditioner for the variable-viscosity Stokes system [69] has been developed. The code was restructured to use language features of Fortran95 and Fortran2003. Using doxygen, an automated code documentation has been integrated. The free-slip boundary conditions and propagator matrix benchmark tests have been investigated. Peter Bollada and Rhodri Davies showed that adding boundary terms to the right hand side of the momentum equation reduces some sort of errors while other kinds of error still exist. They will continue to figure out the exact cause of that behavior and work on fixing this.

After fruitful discussions about possibilities to proper formulate the variable viscosity operator in Terra, Peter Bollada (Leeds), John Baumgardner (San Diego, USA) and Christoph Köstler (Jena) figured out in which way the code has to be changed to apply a physically consistent A-operator using cell-averaged viscosities. The most significant code change is the switch from nodal based to triangle based operator parts on the sphere. The viscosity-weighted summation over triangular integrals is then done in the application of the operator. We expect that the cost for applying $A*u$ will be doubled but a consistent formulation on all grid-levels could pay off for this, especially if we get a better convergence rate of the multigrid algorithm. J. Baumgardner found small missing terms in the current variable-viscosity formulation of Terra and outlined several approaches to pull viscosity out of the derivatives. He made further progress in scaling the momentum tensor and in using local spherical coordinates.

We are going to further improve the parallelization of the particle tracking routines in Terra. Compared to previous Terra versions, there is an extra need for communication among several MPI-processes to figure out connected regions of partial melting in the mantle from which incompatible elements are extracted and transported to the surface. A similar communication is required to define the extent of continents. With the high number of tracers, it is crucial to compress the required global information locally before it is exchanged among neighboring processors. R. Hendel will continue to reduce the communication overhead for tracking globally connected regions, so that the scalability of the particle routines will be extended to 500 and more processors.

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