# First Steps Towards Modeling a Multi-Scale Earth System

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Recent advances in computational geodynamics are applied to explore the link between Earth's heat, its chemistry and its mechanical behavior. Computational thermal-mechanical solutions are now allowing us to understand Earth patterns by solving the basic physics of heat transfer. This approach is currently used to solve basic convection patterns of terrestrial planets. Applying the same methodology to smaller scales delivers promising similarities between observed and predicted structures which are often the site of mineral deposits. The new approach involves a fully coupled solution to the energy, momentum and continuity equations of the system at all scales, allowing the prediction of fractures, shear zones and other typical geological patterns out of a randomly perturbed initial state. The results of this approach are linking a global geodynamic mechanical framework over regional-scale mineral deposits down to the underlying micro-scale processes. Ongoing work includes the challenge of incorporating chemistry into the formulation.

For this, we use computational experiments on micro-scale processes and build a Preliminary Reference Earth Material Database PreMDB. Gibbs energy minimization techniques are used to solve equilibrium compositions

H. Xing, *Advances in Geocomputing*, Lecture Notes in Earth Sciences 119,
DOI 10.1007/978-3-540-85879-9_1

in chemistry and to predict the basic mechanical properties from chemistry. Physical properties that cannot be extracted directly from the thermodynamic potential functions are complemented by empirical data. The next level of models concerns itself with a homogenization of the mechanical properties to larger scale reproducing micro-chemical and microstructural observations. The predictive power of these models is currently tested based on field data from mineral deposits at micro-decameter scale. The next steps will be to upscale the approach to meter and kilometer scale. The global scale modelling will provide better forward simulations for the genesis of giant ore/mineral deposits and other processes of global interest. The approach presented here is intended as a first step for such future cross-scale simulations in geology. Advanced multi-scale formalisms are beyond the scope of this paper.

## 1 Introduction

When applying laboratory data directly to Earth System modeling it is impossible to reproduce key observations and investigate a number of apparent paradoxes, such as:

(1) The subduction initiation paradox; the generation of weak translithospheric faults requires special pleading in classical models (McKenzie, 1977).
(2) The Brace-Goetze (Christmas tree) crustal strength paradox; the continental lithosphere is found to be too strong. Cold continental breakup (for surface heat flow < 60 mW/m$^2$) is not possible under normal geodynamic forcing (Kusznir and Park, 1984a).
(3) The mid-crustal detachment paradox (Axen and Selverstone, 1994); weak crustal detachments are observed exactly where classical strength envelopes predict a strength maximum.
(4) The jelly sandwich paradox (Jackson, 2002); the upper mantle fails to present significant strength and does not deform in a seismogenic manner.
(5) The upper plate paradox (Kusznir, 1991; Weinberg et al., 2007); the brittle crust is deforming much less than the ductile lower crust and mantle.

These paradoxes prompt us to rethink about simple extrapolations of the laboratory strength estimates. Clearly we must improve in our way of modeling the lithosphere. We postulate here, that most, if not all these paradoxes are derived from the fact that numerical models do not take into account feedback effects within a fully coupled momentum-energy-continuity system. We will show that the feedback between deformation, heat production and the mechanical response of the system can resolve these paradoxes. Additional feedback (e.g. melt generation, fluid release) might be important,

but are not required to resolve the paradoxes and are therefore considered to be future refinements. Here we will formulate only a simple formulation showing that this necessarily leads to a multi-scale approach.

## 2 Multiscale Non-Equilibrium Thermodynamics

### *2.1 The Equilibrium Yardstick*

Predicting the way the Earth works from a fundamental physics based approach is a present challenge in computational geophysics. At conceptual level, many approaches have been suggested (Ben-Zion and Sammis, 2003; Fleitout and Froidevaux, 1980; Ord and Hobbs, 1989; Regenauer-Lieb and Yuen, 2003; Yuen et al., 1978), but there has been no development of a clear roadmap for the practical implementation of this approach.

The key to coupling length and time scales is the identification of specific scales relevant for Earth dynamic processes. Candidate for the large scale is the thermal diffusion length scale, which potentially provides a minimum equilibrium yardstick equivalent to a quantum energy state for earthquakes. Microstructure evolution on the other hand relies on a much smaller scale which is of the order of the chemical diffusion length scale. This suggests that thermal-mechanical modelling must explore the equilibrium of these chemical gradients. The chemical diffusion length scale may become the dominant equilibrium yardstick. Although considerable work has been devoted to exploring these approaches in the past, the science of multi-scaling in thermodynamics has not yet made a breakthrough in geology. This is chiefly because coupled thermodynamic modelling is computationally demanding and has not yet become state of the art in the geosciences.

The coupled energy approach has its natural antecedents in planetary scale convection simulations. Figure 1 shows that the same approach applied to smaller scales is promising for exploring pattern formation at these scales. At the large planetary scale, pattern formation is calculated by solving the problem of how a planet looses heat. It is well known that such a planet can reach a critical energy state where convection transfers heat more efficiently than conduction. This occurs when the positive feedback given by the product of buoyancy forces and heat advection overcomes the negative feedback defined by the product of viscous forces and heat conduction. A fully coupled momentum-energy-continuity equation calculation can resolve this instability. Nonlinear feedbacks lead to the onset of convection, meaning that convection emerges self-consistently. The important and underlying assumption for calculating this phenomenon is that any scale(s) below the dominant wavelength for growth of Rayleigh-Taylor instabilities are unimportant for the evolution of these instabilities. Processes

at this scale are approximated by an effective viscous rheology. The dominant wavelength for Rayleigh-Taylor becomes the equilibrium yardstick for calculating planetary convection. Note that this distinction of scales is arbitrary; other scales may just not be resolved and therefore parameterized in the model and they could be still important. However, this approach is now well established in computational geodynamics.

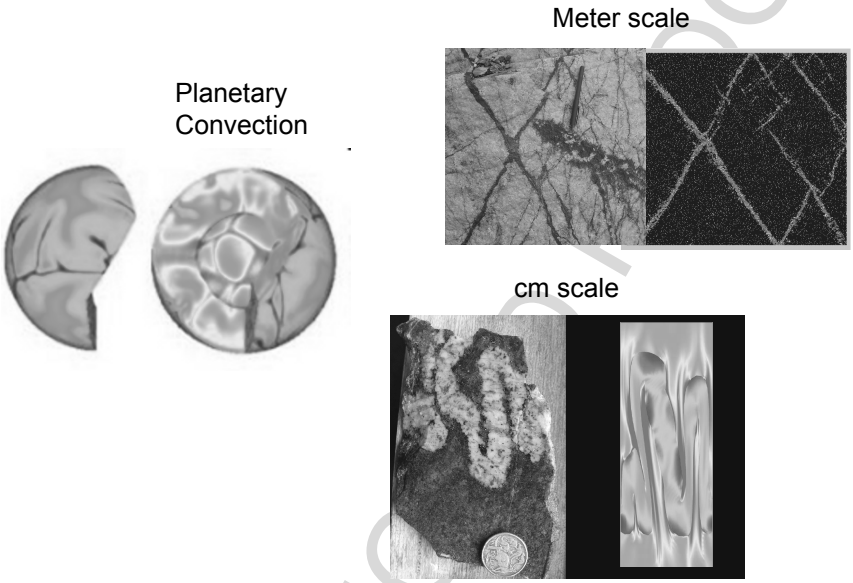


**Fig. 1** Far from equilibrium processes and Earth patterns. Computational thermal-mechanical solutions are now allowing us to understand pattern formation from consideration of basic physics and chemistry. However, a common framework is still lacking. The planetary convection simulation shows the temperature field inside the Earth as resulting from a spherical geodynamical mantle convection model (Bunge et al., 1997). We are proposing here to derive similar Earth patterns at smaller scale emerging out of random perturbations of the basic energy fluxes. Our, first such thermal-mechanical self-consistent results are compared with structures observed in nature. Photographs show conjugated Cu-veins and a cm scale fold (courtesy of Yanhua Zhang and Andy Tomkins, respectively). The attached movie material (Gosford.avi + fold.avi, available on accompanying DVD) show simulation of meter scale fracturing of Gosford sandstone and cm-scale folding, respectively. The Gosford movie shows a particle simulation where particles cracks either in tension (*red*) or shear (*yellow*). With increasing vertical loading, the primary shear zones emerge through the centre of the specimen, with further damage zones, of similar orientation but of lesser scale, emerging off-centre, and reflecting off the boundaries (Movie courtesy of Yanhua Zhang). The cm-fold shown in the other movie emerge out of thermal-mechanical simulation for an initially perfectly layered feldspar-quartz composite (contours show strain). If thermal-mechanical feedback is switched off, the same simulation shortens homogeneously by pure shear

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Patterns at meter scale can also be obtained by fully coupling the mechanics to the energy equation. The particle simulation in Fig. 1 shows a surprising similarity to fracture patterns observed in nature. Here the equilibrium yardstick is the grain size and it is assumed that there is no property change below this scale. A continuum thermodynamic approach applied to cm scale folding, also leads to convincing results. Here, the equilibrium yardstick is the diffusion of some chemical species. The continuum mechanical approach needs to resolve this length scale and the physics of chemical diffusion in order to calculate the patterns emerging out of shortening a randomly perturbed stratified layer. While these results may be qualitatively appealing they do not provide a unified framework.

### *2.2 Non Equilibrium Thermodynamics and Multiscaling*

Most natural processes are non-equilibrium processes. A local equilibrium assumption can be used as a first step towards a multi-scale computation. The assumption on the local equilibrium is an approximation but it holds for many systems. This assumption is valid if it is possible to distinguish two characteristic time scales, that is, the time required to reach the equilibrium in the entire system and the time required to reach the equilibrium in some volume, which is small compared to the size of a system under study.

A brute force computational non-equilibrium method is a better choice, but it will rely on efficient numerical schemes which allow an adaptive multi-scale resolution. Such methods are under development but are not available yet. The local equilibrium assumption works particularly well on a geological time scale because of the logarithmic relationship between relevant processes and their time scales indicated in Fig. 2. The separation of scales relies on the "multi-physics" nature of their underlying processes, spanning from molecular dynamics at the microscale to continuum mechanics at planetary scales. A detailed description of the underlying processes including a summary of numerical approaches can be found in Tables 1, 2 in (Regenauer-Lieb and Yuen, 2003). The large separation of scales has led to a separation of scientific disciplines which are: nanochemistry dealing with atomic scales; structural geology and laboratory physics for analysing microstructures at grain size scale; field geology, structural geology and seismology for analyzing fold and fault length scales; geodynamics for plate tectonic scale and planetary physics for planetary convection scales.

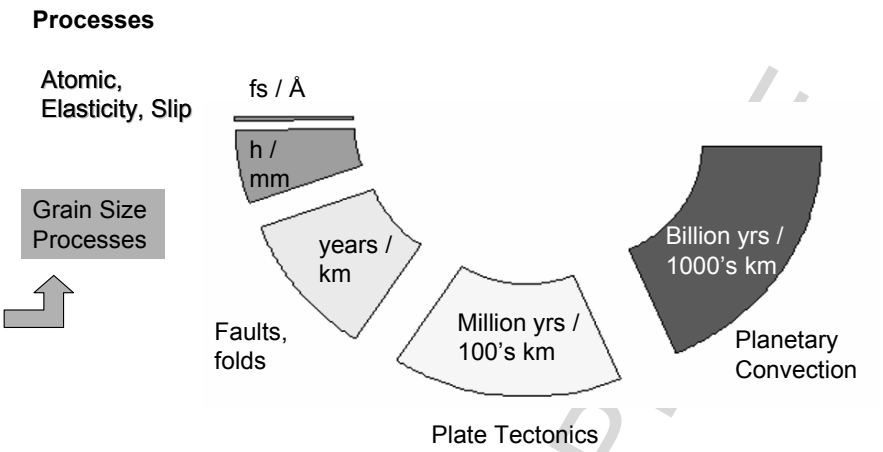


**Fig. 2** Time and spatial processes are coupled. For the equilibrium calculation of elastic constants, time steps of molecular dynamics simulations are on the order of half a femtosecond and the spatial scale is on the order of Angstrom resolution. At the grain size scale with hours of deformation, these elastic properties may be assumed to have reached local equilibrium but faults are out of equilibrium. The same principle may be applied in a staggered sense to the larger plate tectonics and planetary convection scales. An example is highlighted in the figure, namely that of grain size elasticity observed in the laboratory over time scales of seconds to hours, where it can safely be assumed to be in equilibrium. As a simple approach we suggest to derive equilibrium properties for the next larger scale by relaxation to equilibrium calculations at the smaller scale.

The staggered solution method presented here is conceived as the most basic approach towards crossing the traditional scale separations. In doing so the mathematical approach to "multi-physics" interactions is boiled down to a continuum mechanics framework extended by chemistry introducing heterogeneity at grain size scale. We wish to emphasize that such a framework is at best applicable to the "real world" by "nudging" of solutions to observations at various scales. This complication arises because the relaxation to equilibrium at small scale is a function of the large scale hierarchical driver, i.e. different local equilibrium states exist for different large scale out of equilibrium boundary conditions. This important macro-microscale feedback is not yet implemented. The approach is, intended as the first step towards a "heterogeneous multi-scale method" (Enquist and Huang, 2003) which would overcome the deficiency.

### *2.3 Coupling Mechanics and Chemistry*

The simplified local equilibrium approach is a simple avenue for coupling chemistry with mechanics. In order to do so we propose to use local

equilibrium for chemical processes and derive material properties from Gibbs free energy minimization method. Reversible material properties such as thermal expansion coefficient, specific heat, elastic shear modulus, bulk modulus and density, can be directly calculated from this method. These material properties are thus derived self-consistently from thermodynamics.

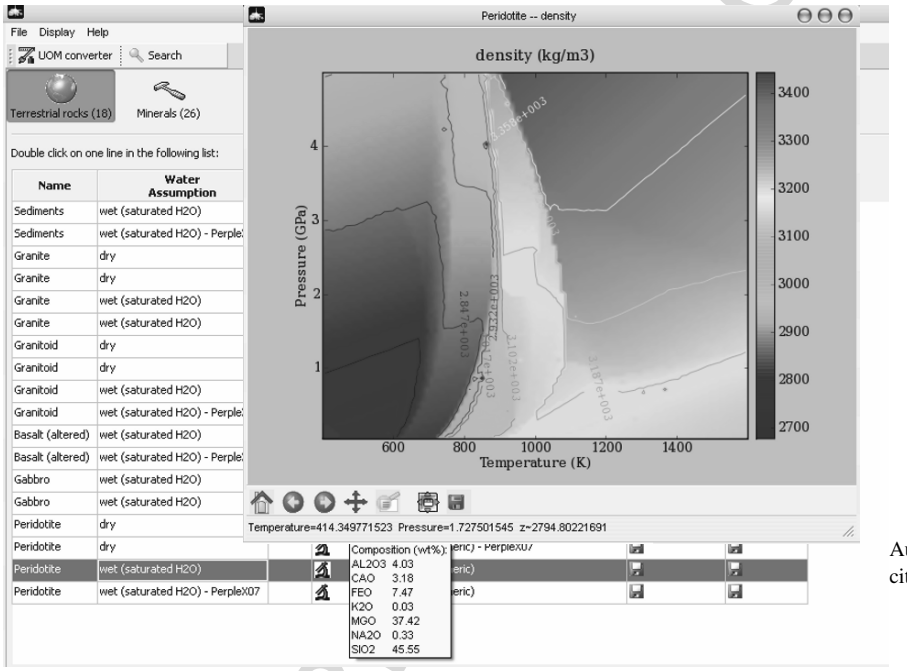


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**Fig. 3** An example of the density at local equilibrium given as a function of pressure and temperature from PreMDB (Siret et al., 2008). The equilibrium density is predicted from Gibbs free energy minimization for the given chemical composition (Peridotite, wet). In addition to density, thermal expansion coefficient, specific heat, elastic shear modulus and bulk modulus can also be derived from the chemical equilibrium

Currently the compositions of 48 major rock forming dry and wet minerals and nine terrestrial rocks have been incorporated into a reference database Preliminary Reference Earth Material Database PreMDB, representing a standard for the sedimentary part of the crust, the upper and lower continental crust, oceanic crust and mantle (pyrolite and peridotite). A total of 20 material properties are obtained and prepared for coupling with finite element models to run non-equilibrium geological, geotechnical and geodynamical models driven by chemical and thermal gradients. Work on an implementation of this chemical solver for larger scales is still ongoing. Of

particular concern is revisiting the behaviour of polyphase rocks as predicted from homogenization calculations of its mineral constituents (Tullis et al., 1991) and its chemical and thermal gradients. The goal of this sub-millimetre (microstructural) – decimetre (meso-) scale work is the derivation of better flow laws for the metre (macro-) scale (Fig. 2). This work is aimed at allowing more realistic coupling of chemistry and mechanics but is not yet completed. In the following we will only discuss plate tectonic scale modelling for which we use empirically derived laws for local equilibrium states.

Non-equilibrium computational models mathematically solve the time dependent evolution of dissipative structures based on maximizing the entropy production. This approach was put forward in the early days of plasticity theory (Martyushev and Seleznev, 2006) where it was called the principle of the maximum specific power of dissipation or the maximum dissipation rate of mechanical energy (Prager, 1959). Ziegler (1983) extended this principle of the theory of plasticity to all non-equilibrium thermodynamics. Numerical methods were not available at the time and it was impossible to calculate dissipative structures on the basis of this principle Therefore the classical developments in continuum mechanics moved away from the early postulates into what is described in the following as a constitutive theory for rock deformation. The two approaches are reviewed in the sections to come. They are labelled "constitutive approach" and "energy approach" respectively.

### *2.4 Classical Brittle-Ductile Modeling*

The Earth's surface deforms in a "brittle" mode represented by pressure-sensitive, temperature insensitive elasto-plastic behavior. The rocks below the brittle-ductile transition (BDT) deform by "ductile" creep represented by pressure insensitive, temperature sensitive visco-elastic behavior. Advanced modeling approaches of the brittle-ductile transition (Albert and Phillips, 2002) employ a combined elasto-visco-plastic approach in which all three behaviors are allowed to occur simultaneously in series. The BDT then emerges self consistently as a narrow transition zone between the plastic (brittle) and the viscous (ductile) regimes above and below, respectively.

While such classical models can reproduce key features observed in large scale geodynamics these numerical predictions fail to reproduce observations on the brittle-ductile transition from microstructural and laboratory analyses. These call for the existence of a broad transition zone named "semi brittle" (Kohlstedt et al., 1995). The semi-brittle regime is the region where brittle and ductile processes overlap. It is thought to be around 10 km wide (Kohlstedt et al., 1995). It is therefore

inferred to be considerably wider than the sub-kilometer scale inferred by numerical models. A second important problem is that in the classical numerical models localized shear zones are mainly driven by brittle deformation while in geology the importance of mylonitic ductile shear zones is very well documented (Christiansen and Pollard, 1997).

Finally, the traditional approach to modeling crustal deformation is based on the balance of momentum with no attempt to consider energy dissipation within the system as a key to solving the "mechanical" evolution of state. Dynamic, time dependent processes, driven by the energy fluxes occurring during an earthquake, for example, are never considered in these approaches. These incompatibilities of observations, nomenclature and fundamental theories form well recognized communication gaps between geodynamicists, rock mechanicians, field geologists, and seismologists (Handy et al., 2001), and a unified approach is needed. This approach is a non-equilibrium thermodynamics formulation (Regenauer-Lieb and Yuen, 2003) which is based on stored and dissipated energy potentials and the principle of maximum entropy production. The mathematical formulation is relatively compact in terms of non-equilibrium thermodynamics and it allows for the incorporation of chemistry. However, since we have not yet routinely implemented the chemical potentials we choose to present the thermo-mechanical formulation in order to relate the two approaches and show the similarities and the differences between them.

We differentiate between two basic modeling strategies for localization phenomena: (1) The classical "constitutive approach", basically a mathematical/engineering approach to failure which is ideal for the lifetime of engineering structures and is used as a first order approximation to geological time scale (2) the new "energy approach" which uses basic physics to calculate failure and may be more appropriate for long geological timescales, since diffusion processes control the degree of potential weakening self-consistently. The energy approach features, in principle, a simplified thermodynamic method. However, we refrain from calling it a "thermodynamic model" since the consideration of energy feedback provides necessary but not sufficient conditions for a unified thermodynamic theory which should in the future include chemistry. In the present version of our model many additional feedback mechanisms with their associated energy states are not yet considered (Lyakhovsky et al., 1997). We describe a very basic setup, where only the entropy change through competition between two simple feedback loops; isentropic thermal expansion (Benallal and Bigoni, 2004) and dissipative shear heating (Braeck and Podladchikov, 2007; Gruntfest, 1963; Kaus and Podladchikov, 2006; Ogawa, 1987; Regenauer-Lieb and Yuen, 1998) differentiate the "energy approach" from the classical "constitutive approach". In the discussion, we will show that

this simple difference can resolve all of the above mentioned discrepancies and paradoxes.

## 3 Mathematical Formulation

### *3.1 Classical Constitutive Approaches for the Lithosphere*

The classical constitutive approach assumes scale invariant material behavior and neglects the principle of maximum dissipation which implies neglect of the conversion of mechanical work into heat. In this approach the uppermost part of the crust is commonly represented by Byerlee's law which is essentially a plastic failure criterion (Albert and Phillips, 2002). The lower part of the crust is then represented by a viscous law (commonly power-law creep). Elasticity is sometimes incorporated into these representations; however, for large scale modeling its effect is often neglected. In the most basic approaches, the switch from one kind of behavior to the other is somewhat arbitrarily defined for a given strain-rate and geothermal gradient, where the stress in the viscous material matches that in the plastic material resulting in a "Christmas Tree" distribution of strength downwards through the crust.

Within the context of the Mohr-Coulomb constitutive relation, Byerlee's law implies a zero value for the cohesion and a friction angle of approximately $50^{o}$; the dilation angle is never explicitly stated but, assuming that this dilation angle is not equal to the friction angle, non-associative behavior is implied with the consequence that localization according to the Hill postulate (Rice, 1977) is possible. However for this to happen, Byerlee's law needs to be expressed in a formulation that allows non-associative behavior in a continuum and not as a failure criterion on a single discontinuity. This allows a prediction of brittle faults without the consideration of the energy dissipation.

One problem of this approach is an arbitrary switch between rheologies at a certain predefined strain rate. This can be avoided through the use of an elasto-visco-plastic rheology, where the brittle-ductile transition can adjust to different boundary conditions. However, when applying only this elasto-visco-plastic strain rate addition, without further couplings, invariably narrow transition zones at mesh resolution are obtained.

In contrast to these constitutive models, our energy models employ a single constitutive relation for the entire crust, namely, that of a modified elasto-plastic von Mises potential (Albert and Phillips, 2002; Regenauer-Lieb et al., 2004) with an added power-law creep term. More precisely, in our approach the yield function at low pressure is a Drucker-Prager function growing in a linear manner with hydrostatic pressure to the classical von Mises yield surface. The elasto-plastic rheology is then commonly

extended by adding a non-linear viscous creep constitutive law assuming power-law creep.

$$\dot{\varepsilon}_{ij}^{tot} = \dot{\varepsilon}_{ij}^{el} + \dot{\varepsilon}_{ij}^{pl} + \dot{\varepsilon}_{ij}^{cr}$$

$$\dot{\varepsilon}_{ij}^{el} = \frac{1+\nu}{E}\frac{D\tilde{\sigma}'_{ij}}{Dt} + \frac{\nu}{E}\frac{Dp}{Dt} + \alpha\frac{DT}{Dt}\delta_{ij}$$

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{el} + \left(\dot{\varepsilon}^{pl}\frac{\sigma'_{ij}}{2\tau}\right)_{plastic} + \left(A\sigma'_{ij}J_2^{n-1}\exp\left(-\frac{Q}{RT}\right)\right)_{creep}$$

where $E$ is Young's modulus, $v$ is Poisson ratio and $\alpha$ is the coefficient of thermal expansion. $\tilde{\dot{\sigma}}_{ij}$ is the objective co-rotational stress rate and $\delta_{ij}$ is the Kronecker delta. The plastic yield stress is $\tau$; $A$ and $n$ are power-law material constants. $Q$ is the activation enthalpy and $R$ is the universal gas constant. $J_2$ is defined as the second invariant of the deviatoric stress tensor:

$$J_2 \equiv \sqrt{\frac{3}{2}\sigma'_{ij}\sigma'_{ij}}$$

$\sigma'_{ij}$ is the deviatoric stress, which is defined by:

$$\sigma'_{ij} \equiv \sigma_{ij} + p\delta_{ij}$$

where

$$p = -\frac{1}{3}trace(\sigma_{ij})$$

is the trace of the Cauchy stress tensor, or the pressure.

We thus use the same formulation as in the classical theory, the only difference being that we do not hardwire shear zone formation into a Mohr-Coulomb approach and we consider the conversion of mechanical work into heat. In our approach shear zones do not appear without this energy coupling.

### 3.2 Energy Approach

Processes that operate in deforming rocks are commonly strongly coupled, in that one process has a first order feedback influence on other processes. Such feedback is neglected in the classical *constitutive theory* for rock deformation. This is done through choice of a special rheology, namely non-associated Mohr-Coulomb (labeled constitutive theory in Fig. 4).

Figure 4 illustrates the mathematical framework underlying the feedback of the thermal diffusion process, which is fundamentally important for the emergence of planetary convection in Fig. 1. The same approach can also predict planetary scale shear zones, if shear heating is considered in addition. Therefore, in a simple model at planetary spatial and temporal scales, the thermal diffusion length scale is sufficient. Thermodynamic models gain complexity when considering smaller scale processes.

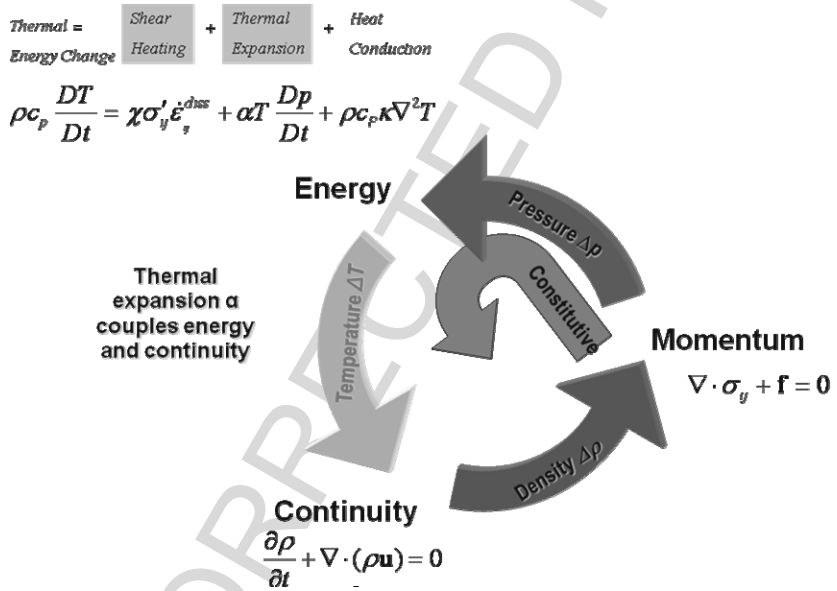


**Fig. 4** Processes in a rock involve small changes in the feedback variables density, pressure and temperature which have a large effect on the deformation of rocks; in particular their localization phenomena. Two key physical processes are described by the two opposing mechanical terms in the energy equation, the dissipated shear heating term (*first grey box* see text for explanation of parameters) and the recoverable, isentropic thermal expansion (*second grey box*). The classical *constitutive approach* bypasses the energy equation and hardwires pattern formation into a constitutive equation

All constitutive equations in our formulation are non-localizing at the outset. However, the rheology must be chosen such that the maximum entropy

production applies. Localization behavior can only arise locally through energy feedback. These energy feedbacks close the balance laws via the energy equation. When investigating the feedback from heat/mechanical power generated through mechanical dissipation two important processes have been identified: (a) shear heating feedback by ductile (viscous) processes assessed through linear stability analyses presented two decades ago (Hobbs et al., 1986); (b) thermal-plastic instabilities arising from elastic thermal-expansion couplings in brittle processes (Benallal and Bigoni, 2004). The latter mechanism is one of a family of mechanisms that incorporate volumetric deformation and density change. Thermal expansion feedback has been found to be a critical phenomenon in experimental studies of the semi-brittle regime (Lu and Jackson, 1998). However, it has only recently been discussed in a thorough theoretical analysis (Benallal and Bigoni, 2004). Now we have the numerical tools (ABAQUS/Standard, 2000; Regenauer-Lieb and Yuen, 2004) available to go beyond the quasistatic linear stability framework with the new approach.

We only use thermo-mechanical coupling through thermo-elasticity and shear heating which leads to flow localization. Thermo-elastic feedback relies on the importance of thermal expansion which in our approach is the only feedback/localization mechanism considered for the brittle field. Shear heating feedback relies on the Arrhenius-temperature dependence of power law creep and is the only feedback loop considered for shear zone formation at greater depth. Thermal expansion feedback introduces weak pressure dependence to the constitutive relation which is equivalent to isentropic dilation. This has the effect that the material develops localization on a length scale that complies with heterogeneities in the spatial distribution of thermal expansion. Thus localization is permitted in both the brittle and ductile regimes arising solely from thermal-elastic dilation effects. We interpret the development of localization through this mechanism in the brittle regime as brittle fracturing, whilst localization in the ductile regime corresponds to ductile shear zone development.

It should be noted that this simple formulation can be extended, but does not, as yet, describe brittle fracture near the surface. At the surface, the plastic dilatancy is several orders of magnitude larger than thermal expansion. However, we suggest that our simple approach adequately captures the elementary physics at higher temperature and pressures corresponding to more than about 3 km overburden.

In our approach the brittle-ductile transition (BDT) emerges self-consistently as a region where both feedback mechanisms overlap at approximately the same magnitude. The principal diagnostic difference to the above described constitutive non-associated approaches for the BDT is that there are two, and not just one, mechanisms for flow localization available, a brittle localization and a ductile localization process. The latter

mechanism is missing in the classical constitutive approach and is the reason for its failure to predict the BDT as a wide transition zone.

We use these two processes to address key issues in geodynamics and earthquake mechanics. While other mechanisms clearly exist, the two different principal physical mechanisms, shear heating and thermal expansion instabilities, are found to be sufficient to explain localization phenomena in all materials, other mechanisms clearly exist, but are not considered for simplicity.

Our new approach is summarized in Fig. 4. This figure highlights the difference between our formulation and previous approaches to flow localization. We employ the feedback between the fully coupled continuity, momentum and energy equations which are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \textbf{Continuity equation}$$

where $\rho$ is the density and **u** is the local material velocity vector of the volume under consideration; the second term describes the divergence of the velocity field. The continuity equation incorporates time as a derivative, which is implicitly derived from the evolution of isentropic (thermal expansion) work in the energy equation.

The momentum equation describes equilibrium of forces

$$\nabla \cdot \sigma_{ij} + \mathbf{f} = 0 \qquad \textbf{Momentum equation}$$

where $\nabla \cdot \sigma_{ij}$ is the divergence of the Cauchy stress tensor and $\mathbf{f}$ is the body force.

The energy equation describes the energy fluxes which in our case are

$$\rho c_P \frac{DT}{Dt} = \chi \sigma'_{ij} \dot{\varepsilon}^{diss}_{ij} + \alpha T \frac{Dp}{Dt} + \rho c_P \kappa \nabla^2 T \qquad \textbf{Energy equation}$$

where $c_P$ is the specific heat and $\frac{DT}{Dt}$ is the material derivative of the temperature. The first term on the right side describes shear heating through mechanical dissipative processes where $\chi$ is the efficiency of converting mechanical work into heat ($\chi \leq 1$). The shear heating efficiency of most materials is commonly 85% and 95% for large strain (Chrysochoos et al., 1989). The second term on the right describes the temperature change

through isentropic/recoverable work arising from thermal expansion and the last term describes the temperature change arising from the phonon part of heat conduction with thermal diffusivity $\kappa$.

### 3.3 Scale Dependence of Ductile Shear Zones

Elasto-visco-plastic modelling with feedback includes all ingredients necessary for the investigation of the transient phenomena leading to the self-consistent nucleation of shear and fault zones. The drawback of this approach is that a proper implementation of the multi-level feedback is computationally expensive due to its inherent multi-scale nature. The computational cost relies on the high degree of spatial and hence temporal resolution that is required to resolve feedback. Different homogenization scales apply to different physical processes. These scales may be decoupled if they are sufficiently wide apart and the smaller scale may be assumed to have reached thermodynamic equilibrium within the time scale relevant for the large scale process. If this assumption is true the calculations can indeed be performed independently. We are here proposing such an approach for the plate tectonic scale.

The spatial scale of resolution can be derived from one-dimensional calculations and from theoretical considerations (Regenauer-Lieb et al., 2006a). Up to now the basic progress in this field has been mostly made in metallurgy. However, for metals the intrinsic material length scales of plasticity and thermal feedback (Lemonds and Needleman, 1986) collapses into the micron-scale. This makes the above mentioned separation of scales impossible and the calculations somewhat more complicated. In geology thermal feedback and meso-scale plasticity spreads out owing to the slow deformation and the low diffusivity of rocks. On the question regarding nucleation of shear zones, a separation of the length scales for shear zone formation is a fundamental issue.

The intrinsic material length scale of deformation by dislocations can be shown to govern the width of shear bands in metals (see Aifantis (1987)). The fundamental physics of this length scale hinges on a breakdown of the classical continuum mechanics below a homogenization scale where dislocation can be referred to as "statistically stored dislocations". Below 10 microns the discrete nature of dislocations is felt and there appear so called "geometrically necessary dislocations" which are related to the gradients of plastic strain in a material. Recently, nano-indentation and micro-torsion experiments have given support to this theoretically postulated limit. It was found that it is 200–300% harder to indent at nano-scale than at large scale (see Gao et al. (1999) for a review). The immediate outcome of this is that

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in plasticity there appears an intrinsic material length parameter characterizing the energy of defects. This defect energy governs the strain gradient of plasticity at mesoscale. This strain-gradient plasticity theory recovers at large homogenization scale the power law hardening relationship when a macroscopic population of statistically distributed dislocations is achieved. While this length scale relies on the shear gradients it has been suggested to expand the theory to include a second length scale for stretch gradients (Fleck and Hutchinson, 2001). All of these length scales are below tens of micrometer scale and are below the length scale of interest for geodynamic processes. For the purpose of our calculations we assume that dislocations can be described in a homogenized way by the power law and calculate feedback processes at larger scale.

Each feedback process has its own diffusional length scale in the quasi-steady state limit, if such a limit can be achieved during the deformation. In this respect, the *energy approach* can be expanded naturally for other weakening/strengthening effects such as those arising from chemical reactions. The limit is defined by a characteristic diffusive length scale $l_i$:

$$l_i = 2\sqrt{\frac{\kappa_i}{\dot{\varepsilon}_{\max}}}$$

where $i$ refers to the $i$th weakening mechanism associated with an effective diffusivity $\kappa_i$ .

Considering, for instance, mechanical weakening through the effect of a chemical diffusion process, the mechanical shear zone width, $l_i$, would be expected to be of the order of centimeters or less, because this is a typical diffusion length scale for chemical species in crustal environments. We assume here that there is no porous flow across the BDT, hence temperature must be the fastest diffusion process trailed by chemistry. Therefore, for plate tectonic length scales of kilometers and time scales of millions of years, the main diffusional scaling length is that of thermal diffusion. In this approach a number of heat source terms become very important (radiogenic heat, heat of reaction/solution, latent heat effects of mineral transformations etc.). In the numerical approach discussed above the main large scale mechanism that is capable of supplying a planar heat source important for a plate bounding fault is shear heating. Its associated feedback in creep deformation and thermal expansion is hence the main factor for plate tectonic localization. This thermal-visco-elastic feedback ensures that energy dissipated by the deformation is capable of weakening the material if temperature dependent mechanisms dominate. We wish to emphasize that this mechanism of shear localization in ductile rocks is intended as the most basic approach. A future comprehensive multi-scale approach should additionally include ductile damage and other micro-scale processes.

It is hence obvious that in this approach the ductile shear localization and weakening is limited by thermal diffusion. The advantage of the new approach is that brittle deformation is also linked to temperature through the isentropic thermal dilation effect. In our formulation brittle shear zones are therefore also governed by a length scale that is controlled by the thermal diffusivity which, in the quasi-steady state limit, describes equilibrium between shear heating and cooling by conduction. Assuming representative values of $\kappa_{thermal}$ of the order of $10^{-6}$ m$^2$ s$^{-1}$ and $\dot{\varepsilon}_{\max}$ of the order of $10^{-12}$ s$^{-1}$, $l_{therm}$ for the shear zone is of the order of 1 km for quasi-steady state, which is a reasonable value for a plate bounding mylonitic shear zone.

This length scale is a new aspect of the physics introduced thermal diffusion. It is the fundamental quantity controlling the final post-localization equilibration width of shear heating controlled shear zones (Shawki, 1994; Shawki and Clifton, 1989) when heat conduction and shear heating are in approximate thermal-mechanical equilibrium. It is also the quantity that governs the resolution criteria for numerical thermal-mechanical modeling of shear zones (Regenauer-Lieb and Yuen, 2003). In order to be able to see thermal feedback in a numerical simulation, we need to resolve below the thermal length scale.

Summing up these length scales, we would want to have a maximum element size of the order of tens to hundreds of metre in order to be able to resolve all feedback mechanism within a single numerical analysis. Now, a typical 2-D geodynamic calculation would comprise an area of 1000 km × 100 km. This would imply a minimum of ten million nodes in the calculation, although in practice not all of the model needs to be resolved at such high resolution, if it does not localize. However, it becomes apparent why ductile shear zones are hard to capture in geodynamical calculations. Ductile shear zones are however not beyond the reach of current computers.

### 3.4 Intrinsic Length Scales for Brittle Faults

There are important differences in the intrinsic length and time scales of elastic, plastic and viscous deformation. Visco-plastic deformation is transmitted by the motion of line defects, so it is a rate limited process controlled by atomic relaxation times. Elastic strain relies on electromagnetic waves, so it is determined by electronic relaxation times. The length scale of plastic deformation relies on the size of line defects and magnitude of lattice vibrations. The length scale of viscous deformation relies on thermal and chemical diffusion through lattice and crystal sizes, while elastic deformation relies on electronic (ionic or covalent) bonding only. In the

classical brittle elastic theory the electronic relaxation time can be neglected, thus a time-invariant formulation may be adopted. One may come to the conclusion that the development of a multi-scale brittle theory is simpler than the ductile theory.

This is erroneous because the concept of time enters through the back door, by the evolution of damage during brittle-elastic deformation, which of course, is again linked to the energy/temperature evolution inside a brittle shear zone. For the evolution of brittle damage inside the fault zone it is also important to know how much of the plastic work is dissipated as heat because both together describe the total state evolution inside the shear zone. It is, hence, logical to start with a solution that can describe crack evolution and crystalline slip by dislocation (largely appearing as heat) together. Such theories are emerging now and they are briefly described.

Multiscale computer simulations are now coming up with a totally new dimension and insight into the dynamics and micro-physics of shear zones. The calculations are conventionally first done at atomistic level with say about 100 million atoms displaying the dislocation evolution around a crack tip (Bulatov et al., 1998). In such dislocation-dynamics simulations, computational efficiency is achieved through a less detailed description of dislocations in which atomic degrees of freedom are replaced by piecewise straight lines, and a mesh spacing (a few nanometres) is used that is larger than the crystal lattice parameter. This means dislocation mobility and close-range interactions are not determined as atomic-level processes, but are specified by external parameters known as “local rules”. For this approach to be predictive, atomistic behaviour of dislocation cores has to be integrated into meso-scale dislocation-dynamics simulations. This can be done by a simple step up in scale (Bulatov et al., 1998). A micro-to-mesoscale connection is proposed in which the local rules are derived from the physically occurring dislocation core processes in an atomistic simulation.

The most complete method for spanning the length scales of dynamic simulations is to embed molecular dynamic calculations into larger scale finite element continuum calculations. This has been done for a crack in a silicon slab where five nested computational dynamic regions have been used (Abraham et al., 1998): the largest continuum finite-element (FE) region; the atomistic molecular-dynamics (MD) region; in between the quantum tight-binding (TB) region; the Finite Element-Tight-Binding (FE-TB) “handshaking” region; and the MD-TB “handshaking” region.

Another interesting method for multi-scaling is by going straight from discrete (molecular dynamics) to continuum style calculations without an

intervening discrete element (dislocation dynamics) step. An inter-atomic-based-potential FEM has been developed, that is capable of reproducing stability criteria at both the atomistic and the continuum levels thus providing a fundamental potential framework for the physics of deformation (Li et al., 2002).

While the multi-scale approaches from atomistic to micro-scale are thus growing rapidly for the case of individual cracks, the next level up of describing the behavior of crack populations appears to be still outside the realm of fundamental atomistic based calculations. For the purpose of doing this, in a first step without the rigor underpinned by MD simulations, we introduce some basic assumptions that serve a priori as an empirical framework.

### *3.5 Scale Dependence for Brittle Faults*

Thermodynamic solutions to the problem of brittle shear zone formation will provide insight into the quasi-periodicity of earthquakes while solutions to the ductile shear zones give insights into the problem of cyclic-like nature of plate tectonics. We have shown above that multi-scaling analyses in ductile shear zones are emerging as a new standard in material sciences. However, in the brittle field the multi-scale thermal-dynamic material properties are less well constrained than the ductile properties. From the last chapter it becomes apparent that we cannot resolve the physics of multiple interacting cracks at large plate tectonic scale chiefly because of lack of computer power. Experiments and field observations suggest, however, that the brittle strength of the lithosphere is probably overstated. Significant scale dependence of the brittle properties of rocks have for instance been reported in the literature on brittle rock experiments and their temperature sensitivity see e.g. (Shimada, 1993). In field observation (mine site load bearing jacks) the brittle compressive failure strength of a rock is for instance found to be at least a factor of three magnitude smaller at meter scale than at cm scale (Pinto da Cunha, 1993). Above 1 m there appears to be a statistical satisfactory number of planes of weaknesses in rocks so that the failure strength does not decrease further. Unfortunately, huge testing machines are necessary to obtain mechanical data relevant for the larger scale. The necessity for assessing the large scale has been realized only for the laboratory assessment of friction (Dieterich, 1979). An equivalent approach is lacking for the compressive failure strength of rocks.

On the weight of the above described observations and in the absence of precise data we assume that the characteristic scale of 1 $m^3$ is the homogenization scale and we assume that that rock strength is defined in the high temperature limit by Goetze's criterion (Caristan, 1982) rather than the

Byerlee law (Byerlee, 1978). Our particular emphasis lies on the high temperature rock strength since this is where the largest deviatoric stresses are expected inside the lithosphere.

## 4 Discussion

The observations of multi-scale material strength from different disciplines reported above suggest that classical scale-invariant material property extrapolations might give an upper bound of strength of the lithosphere. Conventionally, laboratory data are obtained at cm scale and may result in overestimations of lithospheric strength when applied to the hundreds of kilometers scale.

In effect, all of the plate tectonic paradoxes reported in the introduction can be assumed to result from the overestimation of the dynamic strength of the lithosphere by constitutive methods. We briefly summarize results from the "energy approach" which overcome these shortcomings.

The first observation concerns the subduction initiation paradox and the generation of weak trans-lithospheric faults (McKenzie, 1977). This observation required special pleading for classical strength models. It is conceivable that forcing convergence across fracture zones and at the same time requiring enormously high fluid pressures could initiate subduction (Hall et al., 2003). It can be shown on the other hand that the shear heating feedback becomes critical when allowing for a small amount of water inside the lithosphere (Regenauer-Lieb et al., 2001). Energy feedback thus naturally lead to the development of extremely weak km wide shear zones with an effective viscosity as low as $5 \times 10^{20}$ Pas (Regenauer-Lieb et al., 2001; Regenauer-Lieb and Yuen, 2003) and the weak shear zone need not be assumed a priori.

The Brace-Goetze (Christmas tree) crustal strength paradox (Brace and Kohlstedt, 1980) implies that significant deformation of the lithosphere would be prevented for thermal conditions below 75 mW/m$^2$ in compression and a value of 60 mW/m$^2$ in extension (Kusznir and Park, 1984a; 1984b). While such heat flows are not entirely off limits it would imply that any tectonic activity would be impossible for areas below these threshold values. We know that this is not the case. The Asian intraplate has for instance an average surface heat flow lower than 75 mW/m$^2$ (Wang, 2001). The Brace-Goetze strength profile implies that the Asian continental lithosphere is too strong to be indented by the Indian indenter. Likewise, cold continental breakup such as in Galicia margin would be impossible under normal geodynamic forcing. This paradox is solved by considering weakening through shear heating feedback (Weinberg et al.,

Au: "Brace, 1980" has been changed to "Brace and Kohlstedt, 1980", in order to match with reference. Is this OK?

2007). Specifically, two key feedback effects both related to thermal energy, and natural in geological systems, have been included in large scale numerical models of continental deformation driven by plate tectonics: (a) shear heating, whereby heating around a small strength perturbation leads to decreased viscosity, which triggers increased strain rate thus increasing heating, causing the development of a ductile shear zone; (b) thermal expansion feedback, where the same temperature heterogeneities, lead to pressure fluctuations; regions of temperature decrease lead to a pressure decrease, whereas regions with a positive temperature increase lead to a pressure increase thus, triggering the onset or arrest of brittle failure, respectively. Cross scale calculations including such effects can be performed with sufficient local resolution (100 m) nowadays. The solutions show that there is considerable weakening of the strong layers in continents so that the continents are much weaker than previously estimated.

The mid-crustal detachment paradox (Axen and Selverstone, 1994) implies that weak crustal detachments are observed exactly where classical strength envelopes predict a strength maximum. This paradox is conventionally explained by either high fluid pressure or weak rheologies. However, it can be shown that mid-crustal detachment develop naturally out of energy feedback through its effect on continental strength (Regenauer-Lieb et al., 2006b).

The jelly sandwich paradox (Jackson, 2002) highlights the fact that the upper mantle fails to present significant strength and does not deform in a seismogenic manner – yet in the classical constitutive model it would be expected to be the strongest part of the lithosphere. Our models support the hypothesis that it is indeed time to abandon the jelly sandwich. The implications for upper mantle strength and seismicity can be explained by the efficiency of feedback in the mantle (Weinberg et al., 2007) and the fundamentally different seismogenic behavior of quartz compared to olivine (Regenauer-Lieb and Yuen, 2006). This comparison shows that olivine having a high activation energy for creep behaves in a fundamentally different manner to quartz which has a much lower activation energy. The main difference lies in the efficiency of the shear heating feedback. In quartz shear heating feedback is inefficient and therefore cannot easily cross the scales. This leads to unstable dynamic slip pulses with heterogeneous faults. Olivine on the other hand behaves in a much more stable manner because the efficient weakening by shear heating quickly establishes large scale shear zones. These shear zones are characterized by a quasi-equilibrium of heat production on the shear planes and thermal diffusion away from the shear zones.

The upper plate paradox (Kusznir, 1991) implies that the brittle crust is deforming much less than the ductile lower crust. This mismatch frequently observed between stretching values inferred from surface extension and

bulk crustal thinning can be explained by assuming a priori an exceptionally weak middle crust (Nagel and Buck, 2007). However, the weakness of the middle crustal layer is also a natural feature of the energy feedback at the brittle-ductile transition and below (Weinberg et al., 2007).

While it is always possible to argue for special pleading to explain the individual observations we believe that the weight of the sum of the observations is compelling enough to consider the possibility that the lithosphere can become a lot weaker than previously thought through multiscale feedback processes. We have shown here how we can apply large scale planetary thermal-mechanical modeling techniques to small scale features and have presented a first cut of incorporation of chemistry for future more robust up-scaling methods.

**Acknowledgements** We wish to acknowledge support through the Pmd*CRC, CSIRO, the University of Western Australia and the Western Australian Government through the Premiers Science Fellowship Program. David Yuen acknowledges support from ITR and CSEDI programs of National Science Foundation.

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