

# Science and modelling at all scales

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## Introduction

A good metaphor for the science of modelling at all scales is a Russian nesting doll figuring a portly mother of a big family stackable up to a variable level < 30, commonly known as the “Babushka” (grandmother), probably an aberration of “Matryoshka” (from the Latin “mater”).



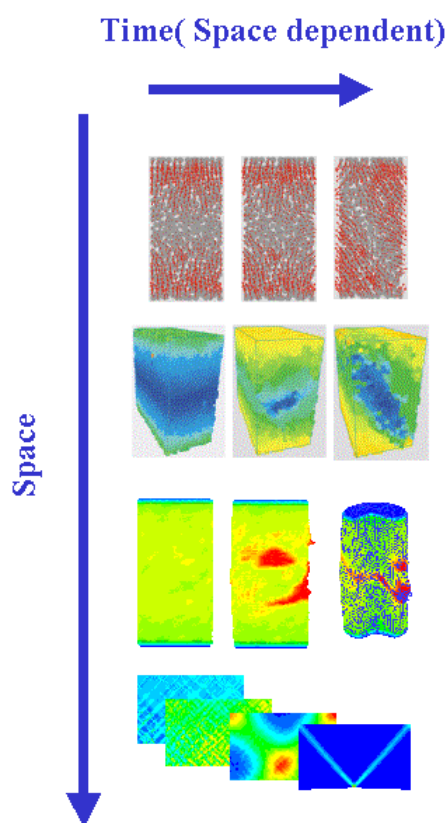
Figure 1. Crossing the scales from brittle microprocesses to planetary-scale convection. The red lines delineate boundaries where new constitutive laws emerge out of spatial averaging of discontinuous processes. Inspired by Kubin’s (2003) unpublished manuscript on electronic to crystal scale processes, which, of course, incorporates a smaller series of Babushkas with its scale dependent physics and mechanical transitions.

While the physics of multi-scaling is reasonably well understood from dislocation to crystallographic level (Moriarty et al., 2002), and for isolated cracks (Abraham et al., 2000), there is a dearth of information crossing the scales from multiple interacting cracks through to the dynamics of fault groups, from the behaviour of plate boundaries to styles of planetary convection. Therefore, up to now, it is common practice to model geological processes by useful phenomenological approaches such as the Coulomb failure criterion, or rate and state variable friction. While this simplification enables a quantitative description of tectonics, the main shortcoming is, perhaps, that it does not lend itself to (or is difficult to implement in) a unified approach coupling chemistry and mechanics. Another criticism is that the phenomenological approach is blind to the scale transitions marked in Figure 1, i.e., it essentially relies on an uncritical extrapolation of laboratory laws to plate tectonic behaviour.

Yet numerical models at local scale need (and are severely influenced by) far field boundary conditions. In the sections to come we briefly describe how we implement a thermodynamic description of the chemical-fluid-mechanical problems. We begin by deriving a self-consistent energy based framework for mechanical porosity by discrete modelling of microcracks. We derive smeared volumes of microcracks to be used at geological terrane scale. Here, we show how scale variant modelling can be simplified at pre-set scales.

### Multiscale-modelling Framework

At the brittle level, we begin with the smallest scale (micron-decimetre scale), and start by compiling results of dilatant rock mechanics laboratory experiments for basic rock types, and reproduce these “ab initio” by particle code (micron - meter scale) (PFC2/3D) calculations. The particle code solves the Helmholtz free energy evolution in a direct way (see Appendix), tracking the local cracking and its self-organization into a shear band. It is subsequently scaled up beyond classical laboratory scale to mining scale observation. At this scale, the discreteness of the individual crack is lost, and crack populations are handed over into their smeared continuum calculations. The smeared continuum calculations are done with classical finite element (FE) methods tracking the Helmholtz free energy fluxes from hundreds of meters - 100 km scale. This part of the project is done in cooperation with Vladimir Lyakhovsky at the University of Jerusalem and is illustrated in Figure 2.



**Figure 2** Top panel: displacement vectors of a particle code simulation of an evolving shear band in a virtual biaxial rock experiment calibrated by a laboratory experiment (see Ord et al., this volume, Fig. 1 and 2, on Gosford sandstone, **Time < 1 hour, Space < 1 m**). Second panel: magnitude of displacement vectors of the same particle code calculation as a spatial average of damage (**Time < 1 hour, Space < 1 m**). Third panel: finite element (FE) damage mechanics calculation of a triaxial rock experiment based on Helmholtz free energy evolution, by V. Lyakhovsky (University of Jerusalem). The dilatancy pattern (damage) mimics the crack evolution of the discrete particle code simulation in a smeared continuum. The FE approach can be applied to the brittle crust scale, while the particle code calculation will be useful to verify the upscaling from laboratory to geological scale. The method is useful for modelling self-consistent dilatancy on shear bands in the brittle part of the lithosphere (**Time < 1 day, Space < 10 km**). Bottom panel: lithosphere-scale, ductile faulting controls the large-scale tectonics. The dissipation contours of lithosphere-scale ductile damage evolving by self-organization of interacting small-scale ductile faults. The birth of this new plate boundary takes less than 100 k years and only occurs if there is an elevated flux of water into the lithosphere. In this calculation, the feedback with the brittle crust has been ignored (**Time < 1 Ma, Space < 100 km**).

At the lithosphere to mantle scale (100 km – 1000 km), fully coupled solid-fluid interaction of lithosphere and mantle is implemented by embedding the FE domain into a boundary element domain for the larger scales. In the future, this model will be coupled to the particle code, thereby obtaining a self-consistent multi-scale geological modeling framework where the different spatial solution routines can in principle be called, based on critical local dissipation. In a first step, we will use a simplified approach and formulate a specific region of interest based on a particle code simulation. We will embed this region within a coupled FEM-BEM method, thus supplying the full feedback between large-scale geodynamic boundary conditions and processes in the local regions of interest.

### **Simplified Modelling at Preset Scales**

Prior to the completion of this software framework, we can use the first results in intermediate solutions and show how modelling can be simplified at preset scales for the purpose of hypothesis testing. The multi-scale framework is useful to add rigour to simplified approaches by exploring the limits of these approaches. If we consider, for example, the crustal scale, we can feed the results from multi-scale modelling back into a simplified phenomenological description. We devise a rheology that satisfies aspects of fault nucleation and weakening. Such a rheology has recently been used to model the genesis of metamorphic core complexes, and is also reproduced in the fully self-consistent energy approach, allowing faulting and core complex exposure to occur through thermodynamic feedback (Wijns et al., work in progress). The fully self-consistent, numerically more expensive simulation is in good agreement with the simplified laws, i.e., it reproduces the same geometric features. The complete approach therefore provides a better base for the simplifying assumptions used. In another example for modelling the Carlin gold trend in northern Nevada, U.S.A. (Wijns et al., this volume), we show how this simplified rheology can be used to test folding/thrusting hypotheses at a local scale. Similarly, at the yet smaller upper crustal scale, we use a simplified reactive transport equation as a proxy for the transfer, dissolution, and precipitation of silica (Sheldon and Ord, this volume). Another simplified approach is presented for the reactive transport modelling of the Mount Isa Copper mineralized system (Kühn et al., this volume).

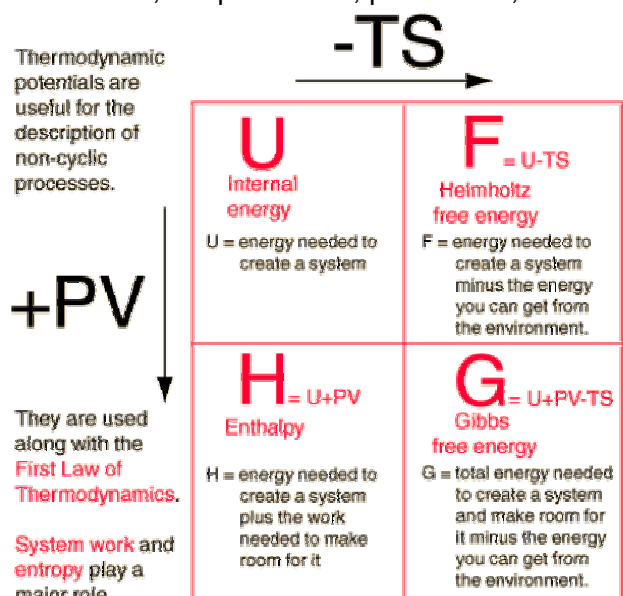
### **Discussion and the Future**

Understanding and explaining emergent constitutive laws in the multi-scale evolution from grain size to plate tectonic scales is making steady progress. Owing to increasing computer power, there have been significant breakthroughs in large-scale geodynamic modelling, which are still awaiting implementation to constrain regional geological modelling. For instance, large-scale convection models have significantly improved to the point of reproducing basic modes of planetary tectonics as self-consistent features of the same physical planetary heat transfer problem (Moresi and Solomatov, 1998; Mulhaus and Regenauer-Lieb, 2004; Stein et al., 2004). The Earth appears to be the only planet known to have developed stable plate tectonics as a means to get rid of its heat. The emergence of plate tectonics out of mantle convection relies intrinsically on the capacity to form extremely weak faults in the top 100 km of the planet, which, in turn, can be related to the critical quantity of water available for thermodynamic rheological feedback mechanisms (Regenauer-Lieb et al., 2004). This explains cycles of co-located resurgence of plate generation and consumption, but also allows a new perspective of lithosphere-scale faults, which in the future shall be used to constrain terrane scale models of massive transfer of mantle volatiles, including reactive transport modelling with upper crustal fluids.

### **Appendix: A Common Thermodynamic Framework for Chemistry and Mechanics**

We summarize the four basic thermodynamic potentials and their interrelation Schroeder, 2000. The thermodynamic potentials are useful in the chemical thermodynamics of reactions and non-cyclic processes, as well as in mechanical modelling. They are the internal energy, the enthalpy, the Helmholtz free energy, and the Gibbs free energy. The four thermodynamic potentials are

related by offsets of the "energy from the environment" term  $TS$  ( $S$  being the entropy, a state variable defining the amount of "disorder" of the system, see second law of thermodynamics) and the "expansion work" term  $PV$ . A mnemonic diagram suggested by Schroeder 2000 can help keep track of the relationships between the four thermodynamic potentials and their state variables:  $S$ , temperature  $T$ , pressure  $P$ , and volume  $V$ .



**Figure 3.** Schroeder's mnemonic thermodynamic diagram can be found as an active graphic on <http://hyperphysics.phy-astr.gsu.edu/hbase/thermo/thepot.html>.

In reactive transport, we minimize Gibbs free energy (for example, HCh or Perplex software), and in mechanical modelling, we describe the fluxes of Helmholtz free energy. Both are related through a transformation (the  $PV$  term). The trend in future modelling will go towards predicting mechanical and thermal properties of materials from thermodynamics. A common framework is already available for water (Wagner and Pruss, 2002). It has been implemented for upper crustal convection (Hornby et al., work in progress).

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