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### **Final Report**

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# Self-Organized Mega-Structures in Sedimentary Basins

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Laboratory for Computational Geodynamics Department of Chemistry Indiana University Bloomington, Indiana 47405 Telephone (812) 855-2717 Fax (812) 855-8300 email ortoleva@indiana.edu http://www.indiana.edu/`lcg The overall theme of the project is to develop a quantitative understanding of basin reaction/transport/mechanical (RTM) processes on a broad range of scales. Our approach starts with the development of novel formulations of the basic RTM process rate laws (e.g. rock deformation, texture dynamics, and fracturing). We then set forth algorithms for solving the resulting partial differential equations numerically. As many of the parameters in the subsurface are not well known, we embed the entire approach in a probabilistic framework through information theory. The result is a set of novel software and conceptual papers that have been the first quantitative theory of a number of fundamental phenomena that take into account the full RTM dynamics of these systems.

We have maintained a focus on self-organization phenomena, a field that we have pioneered for geological systems since the 1970s. In this project we illustrate how diverse phenomena such as oscillatory fault motion, crystal growth, salt diapirism and reaction front morphological instabilities can be understood through self-organization theory. This self-organization initiative over the past several decades has changed thinking in geology and has mainly been under the support of DOE Basic Energy Sciences.

The phenomenon and modeling approaches of this project have many implications for energy resources,  $CO_2$  sequestration, contaminant transport, and waste site remediation. While this project has focused on the geoscience fundamentals, we believe that it has influenced thinking in these areas, notably in the computer simulation of these systems.

A final outcome of this project was that we identified key elements of shorter scale phenomena and modeling that must be addressed if the full predictive power of basin, fault, reservoir and other geoscience modeling is to be achieved. This has been summarized in a follow-on research plan.

In what follows we summarize the individual accomplishments as they are presented in journal articles and two volumes.

# Tuncay, K. and Ortoleva, P. 2001. Salt tectonics as a self-organizing process: a three dimensional reaction, transport and mechanics model. *Journal of Geophysical Research* 106: 803-817.

Salt tectonics is placed within the theory of nonlinear dynamical systems. Features such as waves, diapirs, and tears are viewed as natural consequences of the symmetry breaking instabilities and related self-organized dynamics of the deforming salt body coupled to the reaction, transport, and mechanics (RTM) of the surrounding sediments. The fundamental nonlinearities are in the surrounding-rock and salt rheology. Our findings are based on a 3-D coupled RTM model simulated using finite element techniques. The centerpiece of the rheology of both rocks and salt is a nonlinear incremental stress formulation that integrates poroelasticity, continuous irreversible mechanical deformation (with yield behavior), pressure solution and fracturing. In contrast to previously presented studies, in our approach, the descriptive variables of all solid and fluid phases (stress, velocity, concentrations, etc.) and porous medium (texture, i.e., volume fractions, composition, etc.) are solved from RTM equations accounting for interactions and interdependencies between them. The role of the coupling between the spatial distribution of sediment input rate and diapir growth and stalling are examined as are the creation of an array of salt tectonic mini-basins.

### Tuncay, K., A., Khalil, and P. Ortoleva. 2001. Failure, memory and cyclic fault movement. *Bulletin of Seismological Society of America* 91:538-552.

Faulting is typically a two time scale process--i.e., rapid failure and slow (chemical) healing. Once failed, a rock has a long memory until slow chemical processes have time to re-establish the grain-grain contacts underlying rock competency. The memory of rock failure can be captured by a sufficiently rich textural model and the texture must be coevolved with rock stress and deformation to yield a self-consistent model of strain hardening/weakening, fault narrowing and earthquake cyclicity. A model based on incremental stress rheology and rock texture dynamics is introduced that emphasizes the interplay of rock competency, porosity and other texture variables with stress and strain. The deformation mechanisms taken into consideration are poroelasticity and viscosity. The rheology equations are strongly coupled to the evolution equations of rock texture and pore fluid flow. The model is used to gain an understanding of several oscillatory modes of fault movement. The roles of rock competency, fluid pressure, and continuous deformation in these oscillations is illustrated for various conditions. The approach is shown to be a natural starting point for a theory of the three dimensional, multi-process dynamics of fault nucleation, growth, morphology, reactivation and continuous vs seismic behavior

Tuncay, K., F. Renard, and P. Ortoleva. 2002. Comprehensive 3D modeling of fault dynamics during the seismic cycle. *Poromechanics II*, Edited by J. L. Auriault, C. Geindreau, P. Royer, J. F. Bloch, C. Boutin, J. Lewandowska, Balkema. 947-952. A three-dimensional finite element fault model that accounts for an incremental stress rheology, and fluid and heat flow is presented. In the model, mass and momentum balances for solid and fluid phases, and a total energy conservation equation are solved numerically along with a state and rate dependent friction law at the fault surface. The model allows one to study the effect of frictional heating, fluid influx from the deeper parts of faults, effect of heterogeneities on the fault behavior at the crustal scale.

# Tuncay, K., A. Park, and P. Ortoleva. 2002. Fractures, faults, and the nonlinear RTM dynamics of sedimentary basins. *Resource Recovery, Confinement, and Remediation of Environmental Hazards, Institute of Mathematics and its Applications.* Editors: John Chadam, Al Cunningham, Richard E. Ewing, Peter Ortoleva, and Mary Fanett Wheeler. Springer-Verlag, New York. 131:131-160.

A unique 3-D computer simulator is used to predict natural fracture network characteristics in the subsurface. The model is based on the numerical solution of rock deformation processes coupled to the myriad of other basin reaction, transport and mechanical (RTM) processes. The model integrates seismic, well log and surface geological data to arrive at a quantitative picture of the distribution of fractures, stress, petroleum and porosity, grain size and other textural information. The core of the model is an incremental stress rheology that accounts for poroelasticity, nonlinear viscosity with yield/faulting, pressure solution and fracturing. In this way it couples mechanics to multiphase flow and diagenesis (through their influence on effective stress and rock rheological properties). The model is fully 3-D in terms of the full range of fracture orientations and the tensorial nature of stress, deformation and permeability, as well as all conservation of mass, energy and momentum solvers. The model is fully dynamic as all rock properties (rheologic, multi-phase fluid transport, grain shape, etc.) are coevolved with the other variables.

# Tuncay, K., J. Puckett, Z.Al-Shaeib, and P.Ortoleva. 2002. Kinetics of pits, outgrowths, and inclusions on coated grains. *Geochimica et Cosmochimica*, 66: 3901-3912.

The development of outgrowths or pits of various shapes on coated grains is explained via a quantitative model of grain growth/dissolution kinetics coupled to evolving grain geometry (morphological dynamics). Grain-coating thinning or fracturing occurring due to nonplanar growth (and consequent grain surface area increase) is shown to underlie an instability to the formation of bumps, or in the case of under-saturated systems, to pitting. Examples of diagenetic outgrowth phenomena on clay-coated quartz are presented. A quantitative model of coupled quartz growth and coating dynamics is shown to imply many features observed in natural systems. Crystal growth anisotropy is shown to strongly influence the morphology of the outgrowths. The creation of inclusions is shown to be closely related to the present morphological instability. These morphological instability phenomena are interesting examples of geochemical self-organization. A steady-state model of the diffusion of solutes across the grain coating is shown to yield a novel nonlinear equation to be solved for the rate of growth of coated grains. This equation leads to a complex dependence of the growth/dissolution rate on saturation (or more generally on the composition of the fluid) in the medium surrounding the coated grain. The feedback between the dynamics of the coating thickness and morphology changes makes the phenomenon of interest here distinct from that arising from the coupling of grain growth and diffusion in the surrounding medium. This makes pits and needles possible even in a well-stirred surrounding medium, a fact of interest in interpreting the geologic record. For example, the present model can explain the development of spike, mushroom, and other outgrowths on clay-coated quartz grains in a sedimentary rock, whereas the classic Mullins and Sekerke diffusion model cannot, i.e., the time scale for eliminating concentration gradients in a pore is much shorter than that for grain growth. Predictions of the model are consistent with observations on quartz when typical values of diffusion, growth rate coefficients, and other parameters are used. In this paper, we emphasize that pitting can be closely related to outgrowth instabilities. If this be the case, then pitted dissolution of feldspars is a likely example. As feldspars dissolve, they commonly surround themselves with a clay coating, often leaving only a ghost remnant of the original growth.

# Tuncay, K. and P. Ortoleva. 2002. Probability functionals, homogenization and comprehensive reservoir simulators. *Resource Recovery, Confinement, and Remediation of Environmental Hazards, Institute of Mathematics and its Applications.* Editors: John Chadam, Al Cunningham, Richard E. Ewing, Peter Ortoleva, and Mary Fanett Wheeler. Springer-Verlag, New York. 131:161-178.

A probability functional method is used to determine the most probable state of a reservoir or other subsurface features. The method is generalized to arrive at a self-consistent accounting of the multiple spatial scales involved by unifying information and homogenization theories. It is known that to take full advantage of the approach (e.g. to predict the spatial distribution of permeability, porosity, multi-phase flow parameters,

stress, fracturing) one must embed multiple reaction, transport, mechanical (RTM) process simulators in the computation. A numerical technique is introduced to directly solve the inverse problem for the most probable distribution of reservoir state variables. The method is applied to several two and three dimensional reservoir delineation problems.

## Tuncay, K. G. Ozkan, and P. Ortoleva. 2003. Interplay of gouge, fluid pressure and porosity in fault zone. *Journal of Geochemical Exploration*, 79: 191-195.

The objective of this study is to demonstrate how fault dynamics may naturally be placed in the context of incremental stress theory, rock textural evolution modeling and standard conservation laws. Casting the fault dynamics problem in this framework naturally introduces rock memory for failure, fluid pressure effects and the autonomous nature of fault evolution. Poroelasticity, nonlinear viscosity and gouge are combined in an incremental stress rheology approach to examine the effect of changes in particle size distribution on fluid pressure in fault zones.

#### Tuncay, K., A. Park and P. Ortoleva. 2003. 3-D coupled basin RTM modeling: Applications to fracture, fault and salt tectonic regimes. *Multidimensional basin modeling*, edited by R. Marzi and S. Duppenbecker, AAPG Discovery Series, No 7, 217-242.

A complex network of coupled reaction, transport, and mechanical (RTM) processes underlies the genesis, dynamics, and characteristics of basins. Prediction of basin evolution is, therefore, outside the realm of simple approaches. In this paper, a comprehensive, 3-D basin model is described that accounts for a full suite of RTM processes. Our model accounts for rock deformation, fracturing, gouge and faulting as well as other processes (multi-phase flow, organic and inorganic diagenesis, texture dynamics and heat transfer). The model accounts for most coupling among these RTM processes and accounts for boundary influences (i.e., the tectonic, sea level, basement heat flux and sedimentation/erosion histories). Basin RTM provides a platform for integrating available data using the framework provided by the laws of physics and chemistry. It is also being used to test new concepts and models in fundamental basin research. To illustrate the importance of coupling and comprehensiveness of the model and their 3-D character, we illustrate the use of our model in fractured reservoir, faulting and salt tectonic regimes. The role of nonlinear phenomena in basin evolution is illustrated.

# Meile, C. K. Tuncay, and P. Van Cappellen. 2003. Explicit representation of 3-D heterogeneity in reactive transport models: Application to bioirrigated sediments. *Journal of Geochemical Exploration*, 78: 231-244.

Existing reactive transport models represent aquatic sediments as one-dimensional systems. These models account for the predominantly vertical chemical gradients recorded by traditional pore water and solid sediment sampling techniques (e.g., cores, dialysis samplers). However, advances in sampling techniques, including the rapid development of in situ microprofilers, are providing increasingly detailed data sets, which highlight the laterally heterogeneous nature of the water-sediment interface. In particular, coastal sediments inhabited by macrofauna exhibit large horizontal gradients in chemical composition and microbial communities. The availability of comprehensive and

multidimensional data sets, along with our growing conceptual understanding of the complex biogeochemical dynamics in sediments, requires more sophisticated reactive transport models that explicitly account for the heterogeneity of aquatic sediments. Here, we present a model that explicitly calculates the effect of flushing of macrofaunal burrows on dissolved chemical species distributions.

#### Park, A. and P. Ortoleva. 2004. WRIS.TEQ: Multi-mineralic Water-rock Interaction, Mass-transfer and Textural Dynamics Simulator. *Computers and Geosciences*. 29: 277-290.

Water-rock interactions in sediments are driven by the state of disequilibrium that persists among solids and solutes due to changing temperature and stress conditions, and advective and diffusive influx and efflux of solutes. Water-rock interactions bring about changes to sediment composition and texture through a complex chemical reaction network. These reactions can be divided into two types: solid-solute and solute-solute. Reactions of solids and solute are kinetic, i.e., they depend on compositions of solids and water, temperature, pore water pressure, and stress. Speciation among solutes are described by thermodynamic relations that depend on water composition and temperature. Both reaction mechanisms, mediated by pore water, are strongly interdependent.

WRIS.TEQ is a comprehensive Reaction-Transport-Mechanical (RTM) simulator that accounts for multi-mineralic water-rock interaction mechanisms of kinetics and thermodynamics, and mass transfer due to advection and diffusion. Moreover, the simulator's dynamic compositional and textural model based on a composite-media approach allows self-consistent evolution of sediment composition and texture due to water-rock interactions. Thus, the program can be used to make reliable predictions of sediment alteration due to water rock interactions at the level it was previously not possible. This article describes the fundamentals of water-rock interaction and composite medium models used in the simulator WRIS.TEQ, and how the program is constructed. The utility of the program is demonstrated by simulated diagenetic alteration of sediments composed of complex mineralogy and heterogeneity.

## Tuncay, K., and P. Ortoleva. 2004. Quantitative basin modeling: present state and developments toward predictability, *Geofluids*, 4: 23-39.

A critique review of the state of quantitative basin modeling is presented. Over the last 15 years, a number of models are proposed to advance our understanding of basin evolution. However, as of present, most basin models are two dimensional (2-D) and subject to significant simplifications such as depth- or effective stress-dependent porosity, no stress calculations, isotropic fracture permeability, etc. In this paper, promising areas for future development are identified. The use of extensive data sets to calibrate basin models requires a comprehensive reaction, transport, mechanical (RTM) model in order to generate the synthetic response. An automated approach to integrate comprehensive basin modeling and seismic, well-log and other type of data is suggested. The approach takes advantage of comprehensive RTM basin modeling to complete an algorithm based on information theory that places basin modeling on a rigorous foundation. Incompleteness in a model can self-consistently be compensated for by an increase in the amount of observed data used. The method can be used to calibrate the transport,

mechanical, or other laws underlying the model. As the procedure is fully automated, the predictions can be continuously updated as new observed data become available. Finally, the procedure makes it possible to augment the model itself as new processes are added in a way that is dictated by the available data. In summary, the automated data/model integration places basin simulation in a novel context of informatics that allows for data to be used to minimize and assess risk in the prediction of reservoir location and characteristics.

# Meile, C., P. Berg, and K. Tuncay. 2004. Species dependent pore water irrigation and its effect on the one-dimensional non-local source-sink description, *Geochimica et Cosmochimica* (submitted for publication).

The burrowing activity of benthic fauna can have a major impact on chemical pore water distributions and solute exchanges between sediments and the water column. In 1D early diagenetic models, biologically enhanced solute transport is usually represented by a mass transfer coefficient, or bioirrigation coefficient,  $\alpha$ . In most model applications, all pore water species are assigned the same  $\alpha$ , or relative differences in  $\alpha$  are assumed to mirror those of the solutes' molecular diffusion coefficients. However, as shown here, the effect of bioirrigation on solute exchange across burrow walls and the sediment-water interface strongly depends on the biogeochemical reactivity of the pore water species. Using a simplified early diagenetic reaction network, we compute 3D concentration fields of major pore water constituents around a vertical burrow, as well as the solute fluxes across the burrow wall. From the results of the 3D simulations, corresponding 1D vertical profiles of  $\alpha$  are derived. The  $\alpha$  profiles show pronounced differences from one solute to another. They are also sensitive to the flushing regime of the burrows and the bottom water chemistry. Dissolved  $O_2$  systematically exhibits the highest  $\alpha$  values, while fast oxygenation kinetics near the burrow wall result in near-zero  $\alpha$  values for Fe<sup>2+</sup>. Therefore, multi-component 1D reactive transport calculations based on a single, speciesaveraged  $\alpha$  profile may seriously misrepresent the effects of bioirrigation on early diagenesis. For nitrate, a species-averaged  $\alpha$  profile may even lead to an erroneous prediction of the direction of the irrigation flux across the water-sediment interface.

### Meile, C., and K. Tuncay. 2004. Scale dependence of reaction rates in porous media. *Geochimica et Cosmochimica* (submitted for publication).

Distribution of chemicals in porous media is affected by transport and reaction processes and their description in reactive transport models is typically based on a continuum approximation utilizing the concept of a representative elementary volume. However, reactions involve direct contact of molecules and/or uptake by microorganisms, both of which occur at spatial scales below the micrometer level. Consequently, inhomogeneous reactant distribution at the pore level may lead to poor estimates of reaction rates. In this study, the validity of the continuum approximation is investigated via a pore scale numerical model. Artificial porous media are generated using an identical overlapping sphere algorithm. By comparison between explicit pore scale simulations and macroscopic continuum approximations, it is shown that inhomogeneous solute distribution within the pores can affect estimates of elemental turnover rates. The error associated with large scale rate estimates depends on the pore geometry, reaction kinetics and macroscopic concentration gradient. This error is quantified for a number of reaction types as a function of porosity and implications for surface processes and microbes are briefly discussed.

# Tandon, K., K. Tuncay, J. Comer, K. Hubbard, and P. Ortoleva. 2004. Estimating tectonic parameters for sedimentary basin evolution: Integration of basin modeling and reflection seismology, *Geophysical Journal International*, Vol 156, 129-139.

A data assimilation approach is demonstrated whereby seismic inversion is both automated and enhanced using a comprehensive numerical sedimentary basin simulator to study the physics and chemistry of sedimentary basin processes in response to geothermal gradient in much greater detail than previously attempted. The approach not only reduces costs by integrating the basin analysis and seismic inversion activities to understand the sedimentary basin evolution with respect to geodynamic parameters- but the technique also has the potential for serving as a geoinformatics platform for understanding various physical and chemical processes operating at different scales within a sedimentary basin.

Tectonic history has a first- order effect on the physical and chemical processes that govern the evolution of sedimentary basins. We demonstrate how such tectonic parameters may be estimated by minimizing the difference between observed seismic reflection data and synthetic ones constructed from the output of a reaction, transport, mechanical (RTM) basin model. We demonstrate the method by reconstructing the geothermal gradient. As thermal history strongly affects the rate of RTM processes operating in a sedimentary basin, variations in geothermal gradient history alter the present- day fluid pressure, effective stress, porosity, fracture statistics and hydrocarbon distribution. All these properties, in turn, affect the mechanical wave velocity and sediment density profiles for a sedimentary basin. The present- day state of the sedimentary basin is imaged by reflection seismology data to a high degree of resolution, but it does not give any indication of the processes that contributed to the evolution of the basin or causes for heterogeneities within the basin that are being imaged. Using texture and fluid properties predicted by our Basin RTM simulator, we generate synthetic seismograms. Linear correlation using power spectra as an error measure and an efficient quadratic optimization technique are found to be most effective in determining the optimal value of the tectonic parameters. Preliminary 1- D studies indicate that one can determine the geothermal gradient even in the presence of observation and numerical uncertainties. The algorithm succeeds even when the synthetic data has detailed information only in a limited depth interval and has a different dominant frequency in the synthetic and observed seismograms. The methodology presented here even works when the basin input data contains only 75 per cent of the stratigraphic layering information compared with the actual basin in a limited depth interval.

### Tuncay, K., and P. Ortoleva. Scaling and steady state dynamics in metamorphic and diagenetic systems (in preparation).

Reaction-transport processes in stressed rocks leads to a variety of phenomena including stylolites and differentiated bedding, pressure seals and metamorphic layering. Under the diagenetic and metamorphic conditions wherein these phenomena arise, there can exist

persistent relationships among the growth/dissolution reactions of the participating minerals. These steady state relationships are derived as natural consequences of a multiple scale analysis of the coupled texture/pore fluid dynamical equations and an examination of the stoichiometry of the participating reactions. A novel reformulation of the reaction-transport/texture equations leads to a framework for efficient computation of the dynamics of diagenetic or metamorphic differentiation patterning and related phenomena of academic interest. Implications for petroleum exploration and production include the delineation of conditions for the creation of banded and other seals and reservoir rocks.

## Tuncay, K., and P. Ortoleva. Role of boundary layers in crystal growth (in preparation).

Fast reactions in the medium from which a crystal growth can lead to an interesting phenomenon wherein mass conservation does not appear to be maintained. It is shown that a careful analysis of the fast reaction limiting behavior implies the existence of a fast kinetic transition (FKT) layer near the crystal surface. The method presented allows one to derive the proper reaction-transport equations and boundary conditions, which are to be solved simultaneously with the equilibrium relations (imposed by the fast reactions) and still maintain mass conservation. As near-surface effects are key to understanding crystal growth phenomena (e.g. oscillatory compositional zoning, crystal habit), these results must be utilized in correctly formulating quantitative models. Our approach corrects misconceptions on these phenomena existing in the literature because they are based on models that do not conserve mass. In contrast, our approach allows for an analysis of these phenomena based on sound physical principles. We discuss applications to carbonate mineral systems. The approach is developed for rather general cases in which the treatment is based on an analysis of the matrix of stoichiometric coefficients defining the network of fast reactions in the medium from which the crystal grows.

## Ortoleva, P. 2004. *Mesoscopic Chemical Physics*. 3 Volume Monograph. In final editing.

In this research monograph we present an extensive review of mesoscopic systems and many novel approaches to the theory of their equilibrium and non-equilibrium behavior. Mesoscopic systems bridge the transitional microscopic and macroscopic scales of space and time. As such, theories of mesoscopic systems must reflect a delicate balance of averaging (to bring out their macroscopic behavior) and the preservation of selected microscopic (atomic) scale behavior (to capture their persistent microstructure). In this sense, the basis of mesoscopic theory lies in a statistical framework wherein it is possible to choose the spatial and temporal scale and associated degree of averaging required for the phenomenon of interest. To meet this challenge, a variety of techniques are presented in this monograph.

Mesoscopic phenomena can be of equilibrium or kinetic character. The former occur in systems that are macroscopically at equilibrium such as for an interface separating two coexisting phases or a macromolecule suspended in an equilibrated host fluid medium. While the overall system is macroscopic, the features of interest (interfaces and macromolecular conformation) are relatively small and hence cannot be described by macroscopic (e.g. extensively averaged) equations. The theory of such equilibrium mesoscopic phenomena has traditionally been cast in terms of an augmentation of the macroscopic free energy using terms in the gradient of the descriptive variables—a Landau-type phenomenological approach. The equilibrium structure of molecules can be addressed by explicitly adding atomic configuration coordinates to the macroscopic theory that, in turn, is augmented by Landau-type corrections. It is found more generally that the inclusion of higher order gradient or integral operator terms into macroscopic equations allows for molecular and lattice structures to emerge spontaneously as temperature or other control parameters change. As structure emerges spontaneously in the space-time patterning of the continuum fields, such approaches might be termed self-organizing field theories. These approaches and their basis in rigorous statistical mechanics are the focus of Volume One of this work.

Kinetic theories are developed in Volume Two based on the aforementioned, augmented free energy approaches and related rates of participating processes. As these rates are zero at equilibrium, the augmented free energy is built into the kinetic ansatz to arrive at a self-consistent phenomenological theory. In addition to these phenomenological approaches, attention is placed on the multiple space-time scaling analysis to elucidate the manner in which the microscopic/macroscopic interplay underlying mesoscopic behavior emerges.

These theories of mesoscopic equilibrium and kinetic phenomena are developed for a range of systems of current interest in chemical physics and, in Volume Three, for natural (i.e. biological and geological) systems. Topics from molecular structure and dynamics to multi-phase systems, biological media, crystals, polymers and glasses are investigated in an attempt to illustrate the range of phenomena that can be addressed using heuristic and rigorous approaches.

#### Ortoleva, P. 2004. Memory and the Self-Organizing Planet. In final editing.

Our planet appears so marvelously structured that one might believe it is unique. Does the earth's capacity for complex organization even explain how it was possible for us to "emerge" from primordial dust, ice and gas? In this volume, we present examples that show that this organization can occur naturally through the laws of physics. This selforganized state of matter and energy is only possible under the moderate thermal and chemical conditions that support solid and macromolecular states of matter. In turn, these states of matter impact a planet's behavior by imparting it with the ability to efficiently retain structural information. This memory is necessary for the development of the many observed levels of interdependent organization.

Planets and other sub-stellar bodies exist in a large range of sizes, overall compositions and energy regimes. As self-organization is the development of order, one might expect that bodies of intermediate temperature are most rich in these phenomena. Planets that are too cold do not permit the chemical reactions allowing for the development of complex molecular and supramolecular structure, while those that are too hot destroy solid state or macromolecular organization. Planet size plays a key role; low gravity does not retain fluids and thus cannot sustain the reactive chemical environment that they support. Excessive gravity destroys structure.

The richness of chemistry is only manifest on planets of supra-critical elemental diversity. Too much chemical diversity can mediate against self-organization in hindering

the emergence of a sufficient pool of any one element to allow for many possibilities to develop. A striking example of this in the context of biodiversity is carbon. For these reasons, complex self-organized structures are most likely to occur on moderate planets of elemental diversity.

The reader is taken on a tour of self-organization phenomena that occur in moderate, compositionally diverse sub-stellar bodies. We show, using a great number of natural examples, that solids and molecular complexity are key to enhancing the self-organization potential of a planet. A variety of physico-chemical self-organization mechanisms are presented.