Patterns in our planet: defining new concepts for the application of multi-scale non-equilibrium thermodynamics to Earth-system science

In its 125th anniversary edition (6 May 2005), the magazine *Science* posed the 25 most important unresolved scientific questions for the next quarter century. Several of these are related to the Earth system, comprising the deep Earth together with its oceans and atmosphere; a non-equilibrium system driven by heat fluxes from both the interior of the Earth and the Sun. It is now understood that the individual parts of this system are tightly coupled, so that even small changes in one can have major influences on others. The complex coupling of physical, chemical and mechanical processes presents some serious challenges to the implementation of modern non-equilibrium thermodynamic concepts. In particular, there are insufficient means to describe conceptually the patterns formed as a result of these processes, and the interaction of processes occurring at different scales is, as yet, poorly understood. Non-equilibrium thermodynamics is an overarching discipline that enables rigorous coupling of diverse phenomena that have hitherto been seen as independent. Although non-equilibrium thermodynamics began to grow in the 1930s (Onsager 1931a,b; Prigogine 1955; Truesdell 1969), it has had something of a resurgence in the physical sciences in recent years, embracing ideas from classical solid mechanics (Ziegler 1983) and stimulated by advances in computer performance. Non-equilibrium thermodynamics has now advanced to a stage where it is beginning to offer a unifying approach to understanding and modelling coupled phenomena and complex systems as a whole.

Here, we are extending the phrase ‘Earth system’ to mean more than the coupling between the surface of the Earth and the hydrosphere–atmosphere, to include coupling with the deep Earth as well. Many of the patterns formed from these processes are in need of good descriptions, and there is a serious lack of understanding of the interactions between processes on different scales, both physical and temporal. Progress is often hampered either by the absence of specific theoretical formulations or by their coupling through efficient numerical models.
Resolving these issues and ensuring a breakthrough in modelling of complex geo-processes will require a concerted effort from the broader geoscience brigade, to engage with the wider scientific community.

The concept of this issue grew from a meeting ‘Patterns in our planet: defining new concepts for the application of multi-scale non-equilibrium thermodynamics to earth system science’ that took place from 12 to 16 May 2008 at Victor Harbor, south of Adelaide, organized under the auspices of the Complex Systems Science Theme of the Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia. Based on the concept of a Gordon conference, the meeting brought together scientists working on a range of physical systems, from biological flows in the Earth’s oceans to brittle fracture networks in its crust. Delegates from the CSIRO Exploration & Mining, Materials Science & Engineering and Land & Water met with academic researchers from across Australia and from the USA, the UK, Germany, the Philippines, Poland, France, Israel and Italy. Thirty-five participants took part in an intensive and wide-ranging workshop, comprising 14 hour-long invited overviews and talks and 16 posters, from leading international experts over a range of multi-disciplinary topics directed towards application of the principles of non-equilibrium thermodynamics to the Earth sciences.

The presentations, based on the five themes of geodynamics, seismology and damage mechanics, fluid dynamics (including atmospheric science), materials science and applied mathematics, allowed plenty of opportunity for wide-ranging and collaborative discussions to overcome these issues, together with an integration session on the last day. Each session was intended to summarize the present state of the art, to highlight new concepts and advances and to explore opportunities for cross-linking to the other themes.

Questions addressed at the meeting included: (i) does feedback from heat generated by mechanical and chemical dissipation lead to self-consistent emergence of structure on the scale of the Earth? (ii) Are there key thermo-mechanical–chemical processes that result in critical temperature ranges for which earthquakes are generated? (iii) Is there a universal mechanism that unites phenomena across scales in fluid, solid and chemical mechanics? (iv) Does such an approach enable us to understand complex processes in the oceans, atmosphere and solid Earth and the coupling between such processes? (v) What are the roles that non-equilibrium processes play in producing spatial and temporal instabilities and patterning in the Earth system?

Speakers talked on a diverse range of topics. For example, fluid flow was discussed in a number of systems, including boundary-layer turbulence in forest canopies and chaotic flows in the oceans and through porous media. A wide span of scales was also covered, from evolution of the Earth’s climate and plate tectonics system to the microscopic processes involved in the flow of granular materials. One recurring discussion topic was the effect of scale as a control on the applicability of different mechanistic approaches.

Further discussion was focused on the need to develop a common ‘language’ to aid interaction between the disciplines; much progress was made on this during the course of the week. The results of discussion were encouraging, and a number of different areas for cross-collaboration were identified, ranging from connectivity statistics in porous media to self-organization of...
heat flow through turbulent media. Overall, it was agreed that the event was a great success and fulfilled expectations, being both challenging and informative. Most importantly, delegates left Victor Harbor with new inspiration and objectives.

This issue is the outcome of that conference, together with contributions from a few who could not attend. The fundamental concepts of non-equilibrium thermodynamics are common to all branches of science, and the essential emphasis here is to present material so that each branch of science can see how others have applied the concepts and how new advances can be made. Most of the contributors to this issue were able to attend the conference, and it is clear to us as guest editors that the spirit of the meeting is very much reflected in the manner in which the papers have been written. In the order that they appear, they address the following issues.

The influence of deformation on the melt extraction process within the Earth is discussed by Brown, with particular reference to information left behind in examples of residual lower crust exposed at the Earth’s surface. Coupling between deformation and melt distribution leads to localization of melt into veins and ductile fractures. It is argued that ductile fractures evolve into dykes and that dykes interact to produce a small number of larger ascent conduits with decreasing depth in the crust.

It is then further shown (Hobbs and Ord) that the system described by Brown displays characteristic size and time scales, optimized through coupled feedback processes that grow at the expense of heat supplied to the system and compete with melt advection. These optimal characteristics coincide with a state of maximum entropy production (MEP) rate.

The idea that joint patterns in rocks arise from reaction–diffusion equations is developed by Ord and Hobbs. Based on a mechanism for the formation of dislocation cell substructures in deformed metals, competition between the diffusion of the densities of cracks that are easy to form and that are relatively difficult to form is shown to give rise to the observed patterns.

Olsen-Kettle and co-workers then explore scale dependency and nonlinearities associated with earthquakes. They suggest that mesh sensitivity in numerical models may provide hidden clues to the underlying physics generating the rich dynamics associated with earthquake rupture. Interestingly, earthquake models with oversized mesh elements that are ill-posed in the continuum limit are shown to display more complex and realistic physics than those for which the deformation is well-posed in this limit. They analyse spatial discretization errors introduced into models with oversize meshes, to show how the governing equations may change because of these error terms and give rise to more interesting physics.

Next, Main and Naylor follow this up by testing the hypothesis that MEP is a potential thermodynamic driver for self-organised criticality in earthquake dynamics. The result is positive, with the caveat that the MEP state is near, but just below, the strict critical point where system memory, in the form of fractal patterns in the strain field, emerges as a consequence of a finite-order parameter.

Zidikheri and Frederiksen employ methods motivated by non-equilibrium statistical mechanics of turbulence to solve an important practical problem in geophysical fluid dynamics, namely the parameterization of subgrid-scale eddies.
needed in large-eddy simulations. The subgrid model represents the effects of the unresolved eddies through a generalized Langevin equation. They show that employing these parameterizations leads to close agreement with high-resolution direct simulation models.

Ackland and Wood then present a simplified model of a coupled planetary geosphere–biosphere, with two species in an evolutionary arms race and with each species evolving extreme behaviour to counteract the other. The result is an apparently stable balance, with the planet supporting a maximum amount of life, in unusually patterned configurations. But this is susceptible to very large correlated fluctuations and extinction events if the balance is disturbed. This arms-race evolution and simultaneous mutual collapse of population is observed even for very small differences in how the species behave. It contrasts with the ‘neutral’ theory of two species evolving to fit the same fixed environment, where the failure of one leads to the success of the other.

The unique thermodynamic state of the Earth’s atmosphere was recognized by James Lovelock more than 40 years ago as an indication for the widespread presence of life, which he later used to develop the Gaia hypothesis. Kleidon starts from this observation and describes how non-equilibrium thermodynamics and MEP should be applicable to the Earth system as a whole. He uses this thermodynamic description to derive first-order trends of the Earth system that would be expected from a thermodynamic system that evolves further away from a state of thermodynamic equilibrium and relates these to the presence and evolution of life.

Geological structures involve complex pore geometries, which directly influence the complexity of geofluid mixing processes. The feedback between the geometrical and phenomenological drivers of system complexity is critical in understanding the evolution of geological systems. Trefry and co-workers introduce a stochastic approach to characterizing the impact of geometric structure on fluid scalar response, particularly relevant for periodically pumped systems that are prototype models for orebody evolution.

What are the connections between geochemical pattern formation and chaotic advection? Metcalfe and co-workers explore this question utilizing the equivalence of Darcy and Hele-Shaw potential flow first to visualize experimentally mixing of stirred potential flows and second to derive a predictive theory. This is a first step towards measurements and predictions for a coupled field model of coevolving flow, concentration and deformation.

Using two-dimensional ‘crushable’ discrete-element simulations, Ben-Nun and Einav demonstrate that the ultimate topology in granular systems undergoing confined comminution is mostly affected by the rules that define the self-organization of the fragment subunits. In uniaxial compression, the emerging ultimate topology is shown to be fractal and generally insensitive to alteration of global index properties such as initial porosity and grain-size distribution. Finally, they show that the fractal dimension is approached irrespective to alteration of the criteria that define when particles crush.

This leads to the contribution by Hunt and co-workers, who draw comparisons between two classical mechanical systems under compressive loading—confined granular media and a system of rigid links supported by springs. Each system is
shown to buckle initially into a periodic deflection pattern. The structural model then evolves into a localized form extending over a finite number of contributing links. Analogies are drawn between this route to localization and the formation of shear bands in granular media.

Judd and Stebler then compare and contrast state estimation and filtering for stochastic and deterministic nonlinear systems. They argue that more often than not, the tracking and forecasting of nonlinear systems have more to do with nonlinear dynamics than with statistics. They conclude that recently developed shadowing techniques show significant promise.

This is followed by the contribution of Stebler and co-workers on stochastic modelling of chaotic systems. They explore methods that allow details of a complex system to be replaced by random forces, and test them in an electronic circuit experiment. They then demonstrate and discuss some limitations of these modelling approaches using numerical simulations. This enables a criterion to be identified, which can be used to decide whether a stochastic model will capture the essential features of a given time series.

Finally, Regenauer-Lieb and co-workers extend Ziegler’s MEP principle to the strong integral form. By maximizing and minimizing the resulting equation, they come up with a new concept for obtaining possible bounds on time-dependent solutions, based on the entropy flux and the dissipative processes underpinning deformation. The proposed bounds (i) provide an additional constraint to classical mechanics, (ii) allow development of material laws entirely based on thermo-dynamic potentials, (iii) predict evolution laws for time-dependent material parameters over geological time, (iv) form the scientific basis for a multi-scale formalism, and (v) offer a unified approach for incorporation of chemistry.

We thank John Finnigan for the scientific and financial support of the CSIRO Complex Systems Theme and Danielle Stevens for organizational support of the conference. We thank Felicity Henning for managing the correspondence with authors and reviewers.

We also thank the Engineering and Physical Sciences (EPSRC) and Biotechnology and Biological Sciences (BBSRC) Research Councils UK for financial support of the conference through the Bath Institute for Complex Systems (Multidisciplinary Critical Mass GR/S86525).

The NANIA EPSRC project hosted a public conference and academic meeting entitled ‘Computer predictions for nature and society: should they be trusted?’ in Edinburgh in September 2008. This was also supported by the Royal Society of Edinburgh and the Scottish Universities Physics Alliance (SUPA; http://www.ph.ed.ac.uk/nania/index.html).

Finally, we gratefully thank all authors and attendees and all reviewers, anonymous as well as named.

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Phil. Trans. R. Soc. A (2010)
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