The aerobic transition as an economic ratchet

Rodrick Wallace

Division of Epidemiology, The New York State Psychiatric Institute, New York, NY, USA

Abstract

Punctuated equilibrium, in the sense of Eldredge and Gould in 1972, and path dependence (Gould in 2002), dominate evolutionary processes, many of whose dynamics can be expressed in terms of interacting information sources (Wallace in 2010). Argument based on Feynman's (in 2000) characterization of information as a form of free energy leads to a close, if inverse, analogy between evolutionary transitions and economic ratchets. Driven by such a 'self-referential' mechanism, increases in available metabolic free energy – via the aerobic transition – led to the eukaryotic transition and to life as we know it. Formal analysis focuses on groupoid symmetries associated with the cognitive processes of gene expression, an extension of the symmetry breaking/making perspectives of physical science into biological phenomena. This suggests that understanding modalities of cognitive gene expression, as opposed to focus on genes themselves, provides the deepest insight into evolutionary phenomena, a perspective at some variance with current simplistic gene-centred views that constrain evolutionary theory.

Introduction

The differences between likely early anaerobic mechanisms and aerobic metabolism are remarkable. Canfield *et al.* (2006) discuss many possible electron donors and acceptors available to early anaerobic metabolisms. For example, the reaction $H_2 + 1/2S_2 \rightarrow H_2S$ produces 21 kJ/mol, while the aerobic reaction $H_2 + 1/2O_2 \rightarrow H_2O$ generates some 241 kJ/mol. The evolutionary transition producing this change in available metabolic free energy enabled the eukaryotic transition to complex cellular organisms. What is the nature of such 'self-referential' evolutionary dynamics (Goldenfeld & Wose 2011)? Here we explore an analogy with economic ratchets (Wallace 2015, Ch. 7) that seems particularly illuminating, adapting groupoid symmetry methods that are associated with cognitive gene expression (Wallace 2012).

Evolution involves at least four factors (Lewontin 2010; Wallace 2010):

1. *Variation*: Across individual organisms at any time, there is considerable variation in structure and behaviour.
2. *Inheritance*: Offspring will resemble their own progenitor or progenitors more than other progenitors.
3. *Change*: Across time, variation in structure and behaviour is constantly occurring in surviving organisms.
4. *Environmental interaction*: Individual organisms and related groups engage in powerful, often punctuated, dynamic mutual relations with their embedding environments that may include the exchange of 'heritage material' between markedly different entities through various means.

Next, many of the essential processes within this structure can be represented in terms of interacting information sources, constrained by the asymptotic limit theorems of information and control theories. Following the arguments of Wallace (2010), it can be shown that

1. An embedding ecosystem has 'grammar' and 'syntax' that allows it to be represented as an information source, say X.
2. Genetic heritage can also be characterized as a 'language', and hence an information source Y.
3. Gene expression is a cognitive process that can be expressed in terms of another information source, Z. Cognition, at base, demands that an entity choose one or a small number of responses to environmental or other signals from a much larger set of those available to it. Choice involves reduction in uncertainty in a formal manner, and implies the existence of an information source (Atlan & Cohen 1998). In addition, cognition is canonically associated with an inherent groupoid structure that generalizes the more familiar idea of a symmetry group (Weinstein 1996). See the Mathematical Appendix for a brief introduction to groupoid symmetries. The argument involves equivalence classes of the paths necessarily associated with cognition (Wallace 2012). The inference is quite direct and will not be presented here to avoid reproduction of material already in the literature.

CAMBRIDGE
UNIVERSITY PRESS

4. Large deviations in dynamical systems are excursions from non-equilibrium steady states (nss) that occur with very high probability only along certain developmental pathways, allowing definition of an information source we will call L_D. See Champagnat *et al.* (2006) for details. The essential point is that, according to the Gartner/Ellis and similar theorems (Dembo & Zeitouni 1998), large deviations are to be associated with quantities $-\sum_j P_j \log[P_j]$ where the P_j constitute a probability distribution (Dembo & Zeitouni 1998). Such sums characterize information sources (Cover & Thomas 2006).

As a consequence, it becomes possible to define a joint Shannon uncertainty representing the interaction of these information sources as

$$H(X, Y, Z, L_D).$$

Phase change

Following Feynman's (2000) identification of information as a form of free energy, an 'entropy' can be defined across a vector of driving system parameters $\mathbf{J}$ as the Legendre transform of H (X, Y, Z, L_D):

$$S \equiv H(\mathbf{J}) - \mathbf{J} \cdot \nabla_{\mathbf{J}} H. \tag{1}$$

Then, in first order, it is also possible to apply an analogue to the Onsager approximation of non-equilibrium thermodynamics in which system dynamics are determined by gradients of S in the components of $\mathbf{J}$ (de Groot & Mazur 1984):

$$\mathrm{d}J_t^i \approx \left(\sum_k \mu_{i,k} \partial S / \partial J_t^k \right) \mathrm{d}t + \sigma_i J_t^i \mathrm{d}B_t. \tag{2}$$

This is a standard construction for which $\mu_{i,k}$ is a kind of diffusion matrix, in this approximation. The last term characterizes stochastic 'volatility': the σ_i are magnitude parameters, and $\mathrm{d}B_t$ represents a noise that may not be the usual Brownian white noise which is supposed to have uniform strength at all frequencies.

Setting the expectations of these equations to zero, it is assumed here, produces a relatively large set of nss, each indexed by some set $j = 1, 2, \ldots, j_{max}$ and each characterized by a joint source uncertainty having value H_j. Noise effects ensure that the nss are not inherently unstable.

Assuming metabolic free energy is available from the embedding environment at some index of intensity ρ, it is possible to define a pseudoprobability for state q as

$$P_q = \frac{\exp(-H_q/\kappa\rho)}{\sum_j \exp(-H_j/\kappa\rho)}, \tag{3}$$

where κ is an index of loss due to thermodynamic Second Law effects. We can iteratively use that pseudoprobability to define a 'higher free energy' Morse Function F (Pettini 2007) in terms of the denominator sum,

$$\exp(-F/\kappa\rho) \equiv \sum_j \exp(-H_j/\kappa\rho). \tag{4}$$

Arguing by abduction from physical theory, changes in ρ will, as in the case of ordinary phase transitions at different temperatures, be associated with profound – and highly punctuated – evolutionary transitions (Eldredge & Gould 1972; Gould 2002). As in the case of physical phase changes, higher values of the 'temperature' ρ will be associated with richer cognitive structures. These transitions, it is important to realize, are indexed by the symmetries of the underlying cognitive gene expression groupoids (Wallace 2012) and define entirely new pathways along which organisms develop. The approach represents extension of group symmetry breaking arguments from physical systems to groupoid symmetry breaking/making in biological systems (Landau & Lifshitz 2007; Pettini 2007). This is no small thing.

Ratchet dynamics

It is possible to formally describe an economic-like ratchet that, although constrained by evolutionary limitations, is usually characterized as a 'self-referential' dynamic. Goldenfeld & Wose (2011) describe the underlying mechanism as involving self-referential dynamics in which the update rules changes during the evolution of the system, a function of its state and history.

The evolutionary 'economic-like' ratchet we propose involves the interaction of metabolic energy cycles and the organisms that utilize them. The simplest way to explore such mechanisms is via an extension of equation (4).

First, assume that the right-hand side of equation (4) can be decently approximated as an integral. Second, suppose that the maximum possible value of H, say H_{max}, is much greater than $\kappa\rho$ as a consequence of entropic loss. Third, suppose that $\rho \to \rho + \Delta$, $\Delta \ll \rho$.

This leads to an expression for the free energy index F of the form

$$\begin{aligned}
\exp\left[-\frac{F}{\kappa(\rho + \Delta)} \right] &\approx \int_0^{H_{max}} \exp[-H/\kappa(\rho + \Delta)] \mathrm{d}H \\
&\approx \int_0^\infty \exp[-H/\kappa(\rho + \Delta)] \mathrm{d}H = \kappa(\rho + \Delta).
\end{aligned} \tag{5}$$

Defining another entropy in the free energy measure F as $\mathcal{S} \equiv F(\Delta) - \Delta \mathrm{d}F/\mathrm{d}\Delta$ allows use of an iterated stochastic Onsager approximation for the dynamics of Δ in the gradient $\mathrm{d}\mathcal{S}/\mathrm{d}\Delta$ (de Groot & Mazur 1984). The resulting stochastic differential equation is

$$\begin{aligned}
\mathrm{d}\Delta_t &= \frac{\mu\Delta_t \kappa}{\rho + \Delta_t} \mathrm{d}t + \sigma\Delta_t \mathrm{d}W_t \\
&\approx \frac{\mu\kappa}{\rho} \Delta_t \mathrm{d}t + \sigma\Delta_t \mathrm{d}W_t,
\end{aligned} \tag{6}$$

where μ is another 'diffusion coefficient', $\mathrm{d}W_t$ represents Brownian white noise, σ determines the magnitude of the volatility, and we use the condition that $\Delta \ll \rho$.

Applying the Ito Chain Rule (Protter 1990) to $\log[\Delta]$ produces the SDE

$$\mathrm{d}\log[\Delta_t] = \left(\frac{\mu\kappa}{\rho} - \frac{1}{2}\sigma^2 \right) \mathrm{d}t + \sigma\mathrm{d}W_t. \tag{7}$$

Invoking the Stochastic Stabilization Theorem (Mao 2007; Appleby *et al.* 2008),

$$\lim_{t \to \infty} \frac{\log[|\Delta_t|]}{t} \to < 0$$

almost surely unless

$$\frac{\mu\kappa}{\rho} > \frac{1}{2}\sigma^2,$$

$$\rho < \frac{2\mu\kappa}{\sigma^2}. \tag{8}$$

The essential point is that there will be an upper limit to ρ in this version of the ratchet. Above that ceiling, other things being equal, $\Delta_t \to 0$.

This mechanism might constrain the maximum possible per cent of oxygen in Earth's atmosphere as a result of the aerobic transition.

Conversely, environmentally driven onset of a negative ratchet may explain patterns of local oxygen depletion in aquatic environments: increase in σ triggers a decline in ρ that in turn increases σ.

Another possible inference, however, might well be that increasing 'volatility' as a consequence of global warming can lower global oxygen concentration, perhaps triggering a downward ratchet to Mars-like conditions. The scenario would involve something like economically driven desertification of the tropics followed, through various mechanisms, by large-scale ocean eutrophication and massive plankton die-off.

Discussion and conclusions

These arguments suggest a mechanism by which, given initially sufficient available metabolic free energy, a self-referential upward ratchet or sequence of ratchets in levels of biological organization – like the famous eukaryotic transition – become possible. It is, however, quite striking that such transitions, in this model, are necessarily associated with, and indeed indexed by, groupoid symmetry changes in the mechanisms of gene expression, bringing a central perspective of physical theory – symmetry breaking – into the study of the most central of biological processes. This observation gives new support to arguments that understanding the modalities of cognitive gene expression, centring on regulation, provides deeper insight into evolutionary and other biological phenomena than does the current narrow focus on genes themselves. Indeed, simplistic gene-centred views constrain research efforts and deform not only evolutionary theory, but our understanding of developmental pathologies and disease processes (Wallace & Wallace 2016; Wallace 2017).

Another central question, as raised by one reviewer, is whether ρ, κ, μ and σ can be directly related to the observable characteristics of Earth or other planets. While an answer is beyond the scope of this paper, which is limited to formal characterization of underlying mechanism, there are some hints in existing data. Figure 1, from Berner (1999), shows an estimate of oxygen concentration in Earth's atmosphere over the last 550 million years, using a sediment abundance model.

Apparently, Earth's oxygen concentration is highly dynamic, depending critically not only on present parameters, but on a path-dependent ecosystem/evolutionary trajectory. Such processes are not predictable without historical data, difficult for Earth and even more so for astrobiology.

For Earth, however, some relevant comment is possible.

Figure 2, from the Scripps O_2 Program (Scripps 2017), superimposes rising carbon dioxide and falling oxygen levels from 1985 through 2016. The decline for oxygen is approximately 19 molecules per million per year. Continuing at this rate of loss, atmospheric oxygen concentration would be cut by a half in only 26 000 years, hardly a deep-time effect.
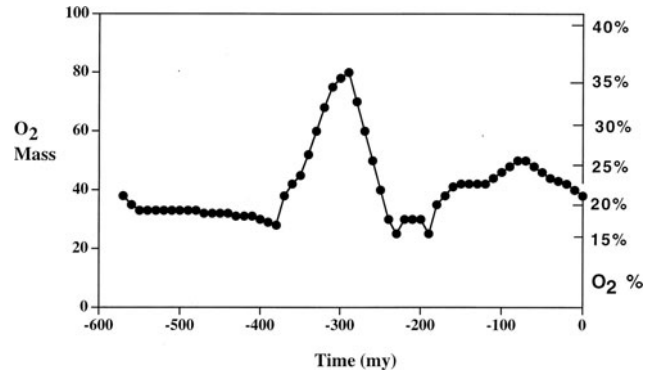

Fig. 1. From Berner (1999). Oxygen concentration dynamics for Earth over the last 550 million years.

Another – possibly synergistic and far more rapid – scenario would be that, under an unregulated 'big business' agroecology, overfarming of tropical landscapes causes widespread desertification, with associated runoff and global climate change that seriously disrupt oceanic phytoplankton life cycles, leading to large, spreading dead zones and triggering a more rapid decline in global oxygen concentration.

Economic-like ratchets, depending on the details, may move in either direction, and can have a broad spectrum of time constants, both matters requiring deeper study than provided here.

Mathematical appendix: groupoids

Given a pairing, connection by a meaningful path to the same basepoint, it is possible to define 'natural' end-point maps $\alpha(g) = a_j$, $\beta(g) = a_k$ from the set of morphisms G into A, and a formally associative product in the groupoid $g_1 g_2$ provided $\alpha(g_1 g_2) = \alpha(g_1)$, $\beta(g_1 g_2) = \beta(g_2)$, and $\beta(g_1) = \alpha(g_2)$. Then the product is defined, and associative, i.e. $(g_1 g_2)g_3 = g_1(g_2 g_3)$, with inverse defined by $g = (a_j, a_k)$, $g^{-1} \equiv (a_k, a_j)$.

In addition, there are natural left and right identity elements λ_g, ρ_g such that $\lambda_g g = g = g\rho_g$.

An orbit of the groupoid G over A is an equivalence class for the relation $a_j \sim Ga_k$ if and only if there is a groupoid element g with $\alpha(g) = a_j$ and $\beta(g) = a_k$. A groupoid is called transitive if it has just one orbit. The transitive groupoids are the building blocks of groupoids in that there is a natural decomposition of the base space of a general groupoid into orbits. Over each orbit, there is a transitive groupoid, and the disjoint union of these transitive groupoids is the original groupoid. Conversely, the disjoint union of groupoids is itself a groupoid.

The isotropy group of $a \in X$ consists of those g in G with $\alpha(g) = a = \beta(g)$. These groups prove fundamental to classifying groupoids.

If G is any groupoid over A, the map $(\alpha, \beta): G \to A \times A$ is a morphism from G to the pair groupoid of A. The image of (α, β) is the orbit equivalence relation $\sim G$, and the functional kernel is the union of the isotropy groups. if $f: X \to Y$ is a function, then the kernel of f, $\ker(f) = [(x_1, x_2) \in X \times X : f(x_1) = f(x_2)]$ defines an equivalence relation.

Groupoids may have additional structure. As Weinstein (1996) explains, a groupoid G is a topological groupoid over a base space X if G and X are topological spaces and α, β and multiplication are continuous maps. A criticism sometimes applied to groupoid theory is that their classification up to isomorphism is nothing other than the classification of equivalence relations via the orbit equivalence relation and groups via the isotropy groups.

La Jolla, California
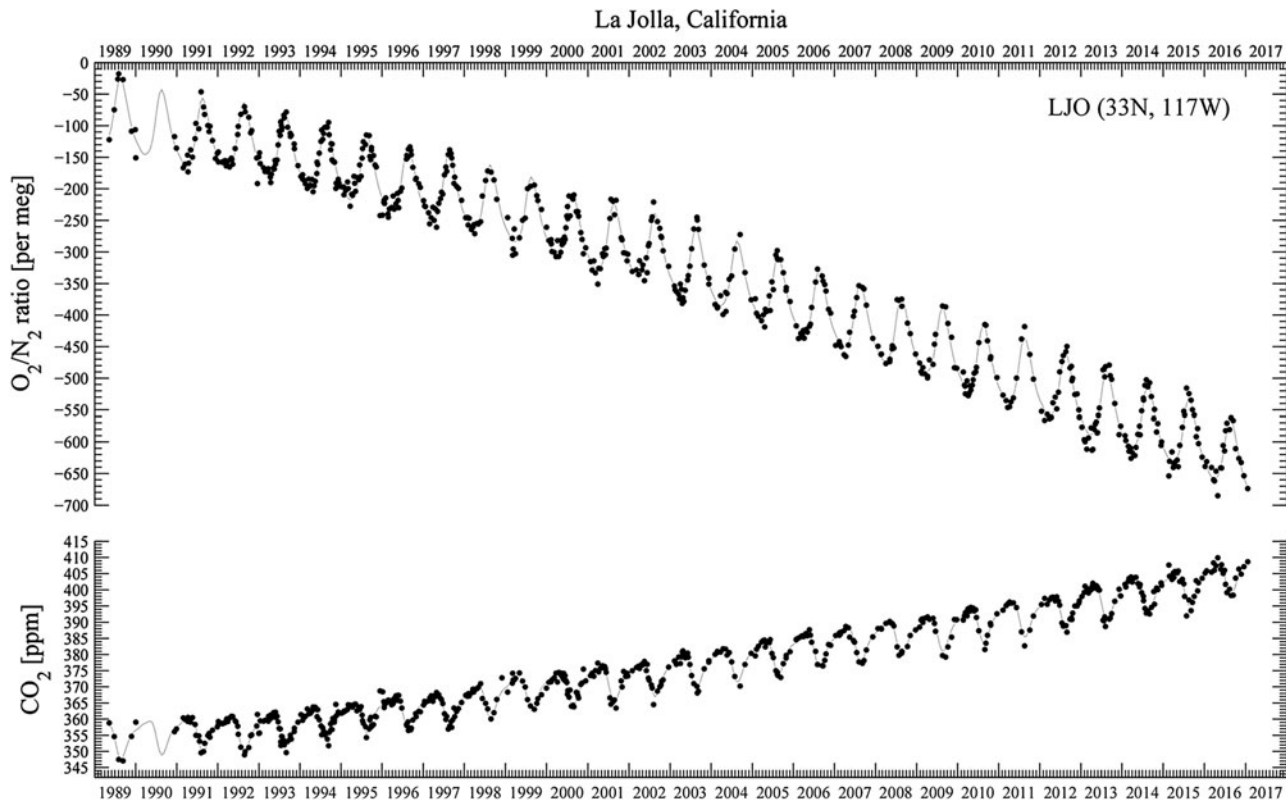
Fig. 2. From the Scripps O_2 Program. Downward trend in oxygen concentration, 1985–2016, and upward trend in carbon dioxide concentration. The upper panel shows oxygen concentrations as changes in oxygen/nitrogen ration in meg units. The lower panel shows carbon dioxide concentrations in ppm units. Points are daily average concentrations, and curves are fit to the data using a spline with a controlled stiffness and a 4-harmonic fit. The falling O_2 level corresponds to losing 19 oxygen atoms per million per year. Atmospheric oxygen concentration, at this rate of loss, halves in 26 000 years.

The imposition of a compatible topological structure produces a non-trivial interaction between the two structures. Below we will introduce a metric structure on manifolds of related information sources, producing such interaction.

In essence, a groupoid is a category in which all morphisms have an inverse, here defined in terms of connection by a meaningful path of an information source dual to a cognitive process.

As Weinstein (1996) points out, the morphism (α, β) suggests another way of looking at groupoids. A groupoid over A identifies not only which elements of A are equivalent to one another (isomorphic), but *it also parameterizes the different ways (isomorphisms) in which two elements can be equivalent*, i.e. all possible information sources dual to some cognitive process. Given the information theoretic characterization of cognition presented above, this produces a full modular cognitive network in a highly natural manner.

Brown (1987) describes the basic structure as follows:

> A groupoid should be thought of as a group with many objects, or with many identities…A groupoid with one object is essentially just a group. So the notion of groupoid is an extension of that of groups. It gives an additional convenience, flexibility and range of applications…

EXAMPLE 1. A disjoint union [of groups] $G = \cup_\lambda G_\lambda$, $\lambda \in \Lambda$, is a groupoid: the product ab is defined if and only if a, b belong to the same G_λ, and ab is then just the product in the group G_λ. There is an identity 1_λ for each $\lambda \in \Lambda$. The maps α, β coincide and map G_λ to λ, $\lambda \in \Lambda$.

EXAMPLE 2. An equivalence relation R on [a set] X becomes a groupoid with α, $\beta : R \to X$ the two projections, and product

$(x, y)(y, z) = (x, z)$ whenever (x, y), $(y, z) \in R$. There is an identity, namely (x, x), for each $x \in X$…

Weinstein (1996) makes the following fundamental point:

Almost every interesting equivalence relation on a space B arises in a natural way as the orbit equivalence relation of some groupoid G over B. Instead of dealing directly with the orbit space B/G as an object in the category S_{map} of sets and mappings, one should consider instead the groupoid G itself as an object in the category G_{htp} of groupoids and homotopy classes of morphisms.

It is, in fact, possible to explore homotopy in paths generated by information sources.

References

Appleby J, Mao X and Rodkina A (2008) Stabilization and destabilization of nonlinear differential equations by noise. *IEEE Transactions on Automatic Control* **53**, 683–691.

Atlan H and Cohen I (1998) Immune information, self-organization, and meaning. *International Immunology* **10**, 711–717.

Berner R (1999) Atmospheric oxygen over phanerozoic time. *Proceedings of the National Academy of Sciences of the United States of America* **96**, 10955–10975.

Brown R (1987) From groups to groupoids: a brief survey. *Bulletin of the London Mathematical Society* **19**, 113–134.

Canfield D, Rosing M and Bjerrum C (2006) Early anaerobic metabolisms. *Philosophical Transactions of the Royal Society B* **361**, 1819–1836.

Champagnat N, Ferriere R and Meleard S (2006) Unifying evolutionary dynamics: from individual stochastic processes to macroscopic models. *Theoretical Population Biology* **69**, 297–321.

Cover T and Thomas J (2006) *Elements of Information Theory*, 2nd edn. New York: Wiley.

de Groot S and Mazur P (1984) *Nonequilibrium Thermodynamics*. New York: Dover.

Dembo A and Zeitouni O (1998) *Large Deviations: Techniques and Applications*, 2nd edn. New York: Springer.

Eldredge N and Gould S (1972) Punctuated equilibrium: an alternative to phyletic gradualism. In: Schopf T (ed). *Models in Paleobiology*. San Francisco: Freeman, Cooper and Co., pp. 82–115.

Feynman R (2000) *Lectures on Computation*. New York: Westview Press.

Goldenfeld N and Wose C (2011) Life is physics: evolution as a collective phenomenon far from equilibrium. *Annual Reviews of Condensed Matter Physics* 2, 375–399.

Gould S (2002) *The Structure of Evolutionary Theory*. Cambridge, MA: Harvard University Press.

Landau L and Lifshitz E (2007) *Statistical Physics*, 3rd edn. Part I, New York: Elsevier.

Lewontin R (2010) Not so natural selection (www.nybooks.com/articles/2010/05/27/not-so-natural-selection).

Mao X (2007) *Stochastic Differential Equations and Applications*, 2nd edn. Chichester, UK: Norwood Publishing.

Pettini M (2007) *Geometry and Topology in Hamiltonian Dynamics*. New York: Springer.

Protter P (1990) *Stochastic Integration and Differential Equations*. New York: Springer.

Scripps (2017) http://www.scrippso2.ucsd.edu/plots.

Wallace R (2010) Expanding the modern synthesis. *Comptes Rendus Biologie* 334, 701–709.

Wallace R (2012) Consciousness, crosstalk and the mereological fallacy: an evolutionary perspective. *Physics of Life Reviews* 9, 426–453.

Wallace R (2015) *An Ecosystem Approach to Economic Stabilization: Escaping the Neoliberal Wilderness*. New York: Routledge Advances in Heterodox Economics.

Wallace R (2017) *Computational Psychiatry: A Systems Biology Approach to the Epigenetics of Mental Disorders*. New York: Springer.

Wallace R and Wallace D (2016) *Gene Expression and its Discontents: The Social Production of Chronic Disease*, 2nd edn. New York: Springer.

Weinstein A (1996) Groupoids: unifying internal and external symmetry. *Notices of the American Mathematical Society* 43, 744–752.