6 Cosmological and Biological Reproducibility: Limits on the Maximum Entropy Production Principle

Charles H. Lineweaver

School of Physics, University of New South Wales, Sydney, Australia.

Summary. The Maximum Entropy Production principle (MEP) seems to be restricted to reproducible dissipative structures. To apply it to cosmology and biology, reproducibility needs to be quantified. If we could replay the tape of the universe, many of the same structures (planets, stars, galaxies) would be reproduced as the universe expanded and cooled, and to these the MEP principle should apply. Whether the concept of MEP can be applied to life depends on the reproducibility of biological evolution and therefore on our ability to distinguish the quirky from the generic features of life. Parallel long term experiments in bacterial evolution can be used to test for biological reproducibility.

6.1 Maximum Entropy Production and Reproducibility

The Maximum Entropy Production (MEP) principle suggests that structures that destroy gradients will arrange themselves such that a maximum amount of entropy is produced (within the given circumstances). On planets, MEP predicts that winds and currents driven by thermal gradients establsih themselves in a way to maximize entropy production (Paltridge 1975, 1979; Lorenz et al. 2001; also several chapters in this volume).

In Boltzmann's derivation of the 2nd law of thermodynamics, the entropy was defined as: $S = k \log W$, where W is the number of microstates by which a given macrostate can be realized. We do not need to describe the microstates accurately and we do not need to know which one of them the system is in, but we do need to be able to count them. In computing the entropy, we are essentially quantifying our ignorance. The system could be hiding in W hiding spots – we do not know which one – so the larger W is, the larger our ignorance and the larger the entropy. In recent ground-breaking work, Dewar (2003) has provided a derivation of Maximum Entropy Production (also Dewar, this volume). Dewar points out that our ignorance can be interpreted as ignorance about anything, not just microstates, and therefore it can be applied to non-equilibrium systems (Jaynes 1957). In Dewar's derivation of MEP, the degrees of freedom are not the number of microstates W of equilibrium systems, available to a particle as in Boltzmann's derivation, but are paths available to the system. To make this conceptual shift we do not need equilibrium but we do need reproducibility, and thus reproducibility becomes the key aspects to whether MEP can be applied.

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Reproducibility can be defined as follows. Let there be two macrostates A and B, each described by only a few parameters. If, each time we set up macrostate A under the same constraints and with the same values of the parameters, it evolves and arrives at B, we call this evolution reproducible. We would like to widen the range of applicability of MEP to cosmology and biology. However, since MEP is limited to reproducible dissipative structures we need to identify such structures in cosmology and biology.

6.1.1 Cosmological Reproducibility

Let us go back to a time 10^{-33} seconds after the big bang and watch another realization of the universe unfold. We will try to identify which structures are produced as they were in our Universe. Which macrostates are reproducible? We assume the same laws of physics, the same constants, forces and the same expansion. The universe begins again hot and dense, and as it expands it cools and rarifies just as it did the first time. As the temperature of the cosmic microwave background (T_{CMB}) falls below the rest masses of elementary particles and the binding energy of protons, neutrons, nuclei, atoms and molecules, these structures form like dew drops condensing out of cooling moist air (Fig. 6.1). Galaxies form again. Stars and planets condense from swirling dissipative accretion disks. Terrestrial planets form with iron cores and wet surfaces. Plate tectonics again slowly stirs and differentiates the crusts while thermal gradients stir up the oceans and atmospheres with currents, hurricanes and cumulonimbus clouds. These dissipative structures are the reproducible products of gravitational clumping and the thermal gradients it produces. We conclude that the MEP should apply to all of them.

6.1.2 The Entropy of an Observable Universe Must Start Low

The big bang model starts with matter and radiation in thermal and chemical equilibrium, and thus apparently the universe begins in a state of maximum entropy or heat death. However, if the universe starts in a state of maximum entropy, entropy cannot increase and any maximum entropy principle becomes an empty statement of initial conditions. Also, since life (and any other dissipative structure) needs gradients to form and survive, the initial condition of any universe that contains life will be one of low entropy, not high entropy. One cannot start an observable universe from a heat death.

The missing ingredient that solves this dilemma is gravity. Matter, evenly distributed throughout the universe, has much potential energy and low entropy. In the standard inflationary scenario describing the earliest moments after the big bang, matter originates from the decay of the evenly distributed potential energy of a scalar field during a short period at the end of inflation called reheating. ‘False vacuum’ decays into our true vacuum. Vacuum energy cannot clump. However, once the potential energy is dumped relatively uniformly into the universe in the form of relativistic particles, these can cool

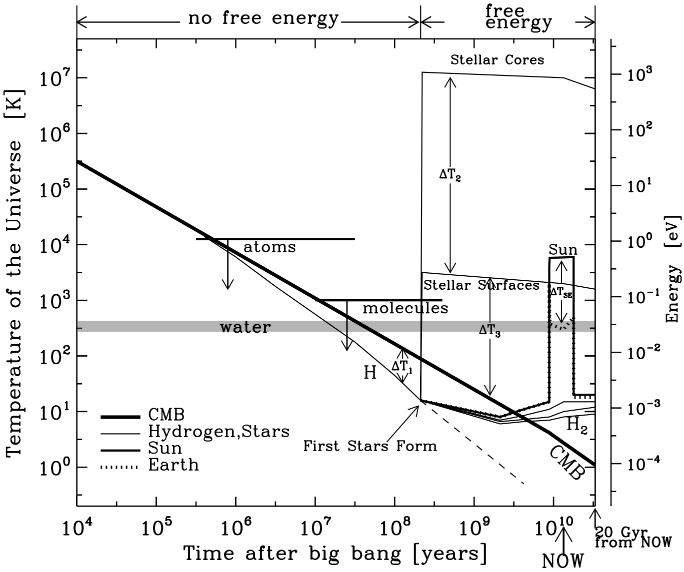

Fig. 6.1. Reproducible aspects of the evolution of our universe. As the universe expands, its temperature (the temperature of the cosmic microwave background "CMB") decreases as: $T_{CMB} \sim 1/\text{size}$. Half a million years after the big bang, the temperature of the universe falls beneath the binding energy of hydrogen. Atoms form. After the formation of neutral hydrogen, matter decouples from the CMB and the temperature of the matter decreases more rapidly than the CMB: $T_{matter} \sim 1/\text{size}^2$. For the first time in the history of the universe, matter and radiation are not in equilibrium with each other. This temperature difference is labeled 'ΔT_1' above. As the hydrogen cools further to $T \sim 20\,\text{K}$, clumps of it gravitationally collapse, heating up and reversing the thermal gradient between the CMB and hydrogen. Star formation begins about 180 million years after the big bang (Bennett et al. 2003). Balls of clumped hydrogen form stars that are $\sim 10^7\,\text{K}$ at their cores and $\sim 10^3 - 10^4\,\text{K}$ at their surfaces. This temperature difference is labeled 'ΔT_2' and is responsible for the convection cells on stellar surfaces as well as for complex stellar magnetic fields. The temperature difference between the surface of the stars and the CMB is labeled 'ΔT_3'. The Sun/Earth temperature difference responsible for all life on Earth is labeled $\Delta T_{SE.}$. The gravitational collapse and radioactivity inside the Earth set up a temperature difference between the center and the surface of the Earth of the same order of magnitude as ΔT_{SE}: 6000 K in the Earth's core and a surface temperature of $\sim 300\,\text{K}$. Thus the gravitational collapse of matter leads to thermal gradients, access to the free energy of nuclear fusion and to all the free energy driving terrestrial life. The current temperature of the CMB is 2.7 K. The energy scale in electron volts on the right helps make contact with the $\sim 0.2\,\text{eV}$ energy scales of the redox potentials that drove the molecular evolution that led to the origin of life (Nealson and Conrad 1999). For example, when ATP becomes ADP, 0.04 eV is released and photosynthesis extracts $\sim 1\,\text{eV}$ from each solar photon

and clump. The gravitational potential energy is enormous – analogous to a homogeneous distribution of boulders at all altitudes through the atmosphere. Thus, in this inflationary picture the potential energy of the vacuum is the ultimate source of all energy and the required low entropy initial state. The energy comes in the form of matter/antimatter pairs which annihilate and create a bath of photons. Because of an intrinsic asymmetry, the annihilation is incomplete and leaves one baryon for every billion photons. Their subsequent cooling (due to the expansion) and clumping of the baryons (due to gravity) is the source of all the free energy, dissipative structures and life in the universe.

6.1.3 Expansion Does Not Increase the Entropy of the Universe

In discussing maximum entropy production in the universe it is important to know what the entropy sources are, whether there is some maximum bound to the entropy of the universe (Fig. 6.2) and whether the expansion of the universe produces entropy.

It is difficult to talk about the total entropy in the universe without knowing how big the universe is. So we talk about the entropy in a representative sample of the universe. Typically we put an imaginary sphere around a few thousand galaxies and consider the entropy in this sphere. As the universe expands so does the sphere whose entropy we are considering. This is called the entropy per comoving volume. We parameterize the expansion of the universe with a scale factor R. This means that when the universe increases in size by a given factor, R increases by the same factor.

The entropy density s of a radiation field of temperature T is $s \sim T^3$. The entropy S in a given comoving volume V is $S = s\,V$. Since the comoving volume V increases as the universe expands, we have $V \sim R^3$. And since the temperature of the microwave background goes down as the universe expands: $T \sim 1/R$, we have the result that the entropy of a given comoving volume of space $S \sim R^{-3} * R^3 =$ constant. Thus the expansion of the universe by itself is not responsible for any entropy increase. There is no heat exchange between different parts of the universe. The expansion is adiabatic and isentropic: $dS_{expansion} = 0$.

If expansion does not produce entropy, what does? Any region of the universe can be considered as an isolated cosmic box. The reason why entropy is increasing is because there are stars in that box. Hydrogen fuses to helium and nuclear energy is transformed into heat. Energy is released at the center of a star at millions of Kelvin and radiated away at thousands of Kelvin (ΔT_2 in Fig. 6.1). Dissipative stars extract energy at high temperature and discard it at low temperature.

To measure entropy in cosmology we just need to count photons. If the number of photons in a given volume of the universe is N, then the entropy of that volume is $S \sim k\,N$ where k is Boltzmann's constant. The vast majority of the entropy of the universe is in the cosmic microwave background. Stars cannot change that. If all the matter in the universe were transformed into 3 K blackbody radiation, the number of photons would add up to only $\sim 1\,\%$ of the number of CMB photons. The entropy of the universe would increase by only 1% .

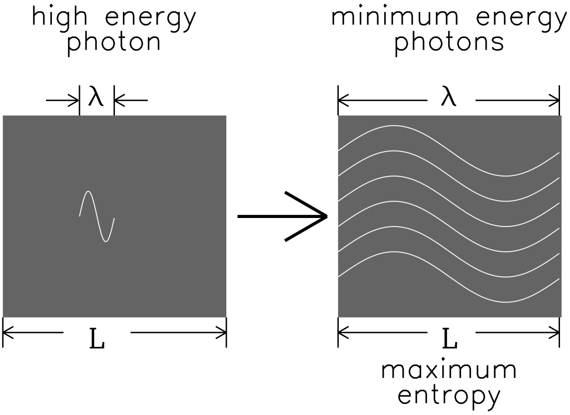

Fig. 6.2. The maximum entropy of the universe. The universe as a whole, or box-like partitions of it, can be treated as a closed system for which $dS \geq 0$. The maximum entropy of a closed system of size L is obtained when all the energy E, within the system is degraded into the smallest bits possible, i.e., all energy is converted into minimal energy photons with wavelengths as large as the system. This is the maximum entropy condition (Bekenstein 1981): $S_{max} = k\,N_{max} = k\,E/E_{min}$, where E is the energy within the comoving volume and the minimum quanta of energy is $E_{min} = hc/\lambda_{max} = hc/L$. Thus, we have $S_{max} = kEL/hc$, and the result is that the maximum entropy of the universe is proportional to the increasing size of the universe: $S_{max}(t) \sim L(t)$ (see Fig. 6.3 for limits on this size)

6.1.4 Return of the Heat Death

Before the discovery that 3/4 of the energy density of the universe was vacuum energy ($\Omega_\Lambda \sim 0.73$), it was thought that the expansion of the universe made the concept of classical heat death obsolete, because in an eternally expanding universe with an eternally decreasing T_{CMB}, thermodynamic equilibrium is a moving unobtainable target (e.g., Frautschi 1982). However, the presence of vacuum energy (also known as a cosmological constant) creates a cosmological event horizon (Fig. 6.3) and this imposes a lower limit to the temperature of the universe since the event horizon emits a blackbody spectrum of photons whose temperature is determined by the value of the cosmological constant:

$$T_\Lambda = 1/2\pi\,\Lambda^{1/2} \tag{6.1}$$

This is the minimum temperature that our universe will ever have if the cosmological constant is a true constant. Current values of Λ yield $T_\Lambda \sim 10^{-30}$ K. This new fixed temperature puts an upper bound on the maximum entropy of the universe and therefore reintroduces a classical heat death as the final state of the universe.

To summarize our cosmological considerations: Galaxies, stars and planets are reproducible structures and should be describable by MEP (see also Sommeria, this volume). The expansion of the universe by itself produces no entropy. Stars are currently the largest producers of entropy in the universe but all the stars in the universe will only ever be able to produce about 1% of the entropy contained in the CMB. The newly discovered cosmological constant limits the maximum entropy of the universe, and consequently the universe is on its way to a heat death.

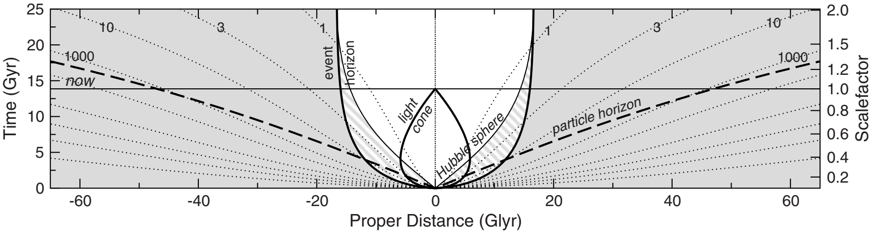

Fig. 6.3. The maximum size L of the system in Fig 6.2 is the cosmic event horizon shown here. As the universe expands the only part of it we can see is along our tear-drop shaped past light cone. As the universe gets older, our past light cone asymptotically approaches the event horizon. Our worldline is the central vertical line. Distant galaxies recede from us along the *dotted lines* – the worldlines of galaxies with currently observed redshifts of 1, 3 and 10 are labeled. Since the energy density of the universe is dominated by a cosmological constant Λ, the universe has an event horizon whose largest radius will be $\sim$ 18 billion light years ('Glyr'). Therefore the longest wavelength photon that will fit in the universe (a photon of the lowest possible energy) will have a wavelength that spans the universe: $\lambda_{max} \sim 36$ billion light years. The cosmic event horizon imposes a maximum physical size to the observable universe and therefore a maximum wavelength of light λ_{max}. Therefore, since $S_{max}(t) \sim L(t) \rightarrow L_{max}$, S_{max} approaches a constant. The temperature of the universe approaches T_Λ and a heat death for the universe is possible ($S_{universe} \rightarrow S_{max}$). In such a situation the energy within the event horizon goes down and one would expect S_{max} to decrease. However, in Davis, Davies and Lineweaver (2003) we showed that the loss of entropy due to loss of energy is compensated exactly by the increasing entropy of the increasing area of the cosmic event horizon (figure from Davis and Lineweaver 2004)

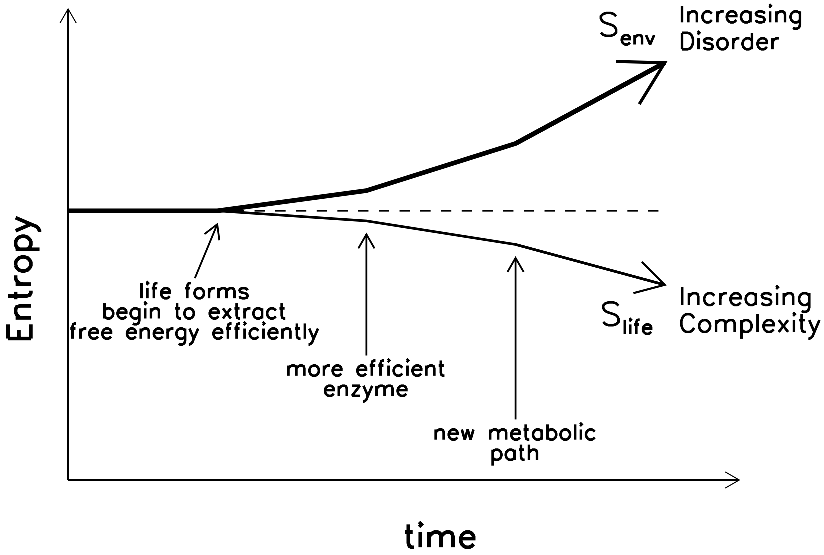

Fig. 6.4. Consider the entropy budget of a dissipative system and its immediate environment (S_{life} and S_{env} respectively). Dissipative systems have a low internal entropy maintained by the export of entropy to the environment: $dS = dS_{life} + dS_{env} \geq 0$. If the system is such that its order is increasing, $dS_{life} < 0$, this necessarily happens at the expense of the environment and we have $dS_{env} > |dS_{life}|$. The decreasing entropy of life does not violate the 2nd law since dS_{env} more than compensates for the lowering of entropy inside life. As life evolves and its metabolic paths become more efficient at extracting available free energy, this should lead to changing slopes as shown in the diagram (see also Chaisson, this volume)

6.2 Biological Reproducibility

6.2.1 Does Life Increase the Total Entropy Growth over What It Would Be Without Life?

Much evidence supports the idea that life increases the rate of entropy production (Fig. 6.4). For example, forests absorb more solar radiation by their lower albedo, and are cooler than deserts at the same latitude and thus produce more entropy. The decreasing S_{life} of Fig. 6.4 represents the increasing complexity of biological evolution. This trend is presumably due to the fact that life forms that can extract more work (and therefore produce more entropy) survive preferentially (Lotka 1922a,b; Ulanowicz and Hannon 1987). Ulanowicz and Hannon (1987) describe this as: “If two systems receive the same quantity of energy at the same entropy, that system which extracts the most work from its input before releasing it to its environment (as it inevitably must) can be said, in the second law sense of the word, to be the more efficient utilizer. Having extracted more work from the given amount of energy, the quality of the release is less, i.e., its entropy is higher." Thus, the evolution of more efficient metabolisms should be equivalent to the evolution of larger entropy production.

Figure 6.4 represents biological dissipative structures increasing net entropy ($dS = dS_{sys} + dS_{env} \geq 0$). We simplistically assumed no change in entropy due to the abiotic processes on the planet (horizontal dashed line). More realistically we need to include the entropy production by abiotic processes on a planet (Fig. 6.5).

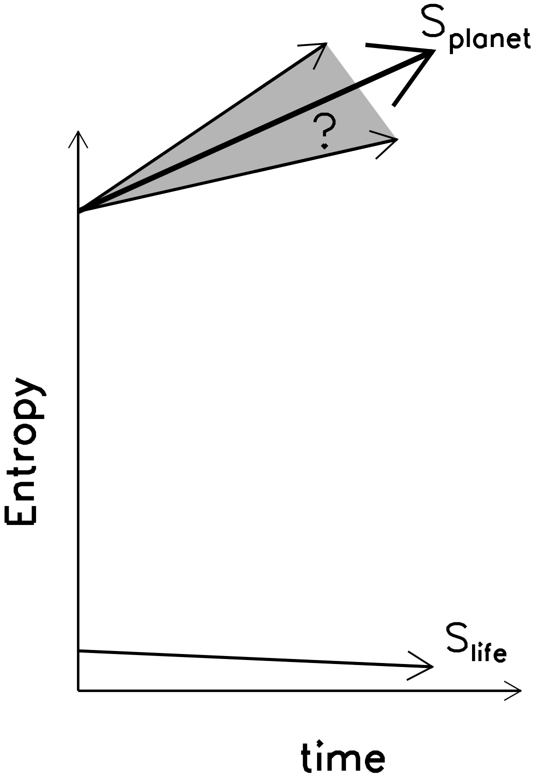

Fig. 6.5. Entropy produced by a planet (and life on that planet) as a function of time. The small decreasing entropy of life is negligible compared to the entropy and entropy production of the planet. If feedback mechanisms regulate the temperature of the planet, life can either increase or decrease the entropy production of the planet (grey region around S_{planet})

The conceptual Daisyworld model of Watson and Lovelock (1983) provides an example to investigate the role of biotic effects on planetary entropy production (see also Toniazzo et al., this volume). In Daisyworld, daisy albedo regulates planetary temperature. The fact that the Sun's luminosity increases on long time scales puts the focus on temperature reduction (= entropy increase). However, a symmetry is assumed, that it is just as easy to increase the temperature as it is to decrease it. Thus the assumption is made that entropy decrease is just as likely to occur as entropy increase. Such feedback mechanisms between dissipative systems are candidates for a violation of MEP if it can be shown that they arise reproducibly. It is still an open question whether such feedback mechanisms are symmetric with respect to entropy production (Ulanowicz and Hannon 1987). The issue is not whether life can make $dS_{planet} < 0$, but whether life can make dS_{planet} lower than it would be without life (under the second law constraint that $dS_{planet} > 0$). In Fig. 6.5, this symmetry and uncertainty are reflected by the symmetry of the grey area around S_{planet} and by the question mark in the case of entropy decrease. This issue is important for proposed resolutions to the faint early Sun paradox, which e.g., invoke biotic methanogenesis to warm the early Earth and reduce its entropy production (Pavlov et al., 2000).

6.3 Applying the Maximum Entropy Principle to Biological Evolution

One problem with applying MEP to life is the identification of the constraints (e.g., Lagrange multipliers). One by one, life can explore and reach out to influence the constraints and one by one the system can modify the previously "external" constraints. If this is happening continuously, then at any one time the current entropy maximum will be a local maximum not a global one, for it will be replaced by a larger maximum as soon as life figures out how to tap into other sources of free energy. This evolution is shown as the slope changes in Fig. 6.4. Since the number and complexity of constraints is large, this process can continue as long as untapped sources of free energy are available. Thus we hypothesize that MEP prescribes stable maxima for non-living dissipative structures and transient local maxima for life (see Kleidon and Fraedrich, this volume, for potential global maxima in entropy production at the planetary scale). In the general debate surrounding Lovelock's Gaia hypothesis (Lovelock 1972, 1988; Lovelock and Margulis 1974) a central issue is whether the biosphere, without other biospheres to compete with, can evolve in a way analogous to the way more traditional units of life, e.g., species, evolve (Lovelock 1988, Dawkins 1982). If competition and natural selection are the only drivers of evolution then the idea of Gaia evolving without competition seems inappropriate. However, if the second law of thermodynamics, in the form of maximum entropy production, can be successfully used to describe evolution, then considering the biosphere as an evolving life form seems more appropriate. In Dewar's derivation, competing micropaths lead to a global state of maximum entropy production. These micropaths, or degrees of freedom, do not have to be realized for the macroscopic steady-state to establish MEP. It also seems that MEP will be established globally independent of whether other Gaias are realized to compete with our Gaia. This contrasts with Dawkins' view that the competitors need to be present for selection to result in the evolution of Gaia.

6.4 Does the MEP Imply That Life Is Common in the Universe?

We would like to know how common life is in the universe. The rapidity of terrestrial biogenesis is sometimes invoked to support the idea that life is common in the universe (Lineweaver and Davis 2002). de Duve (1995) has argued from a biochemical point of view that life is a cosmic imperative. Does the MEP have anything to say on this issue?

Among the structures in the universe, far from equilibrium dissipative structures are ubiquitous and inhabit regions of thermal and chemical gradients (Prigogine 1980). Stars, convection cells, whirlpools, and hurricanes are common. MEP should apply to these reproducible macrostates. The formation of auto-catalytic reactions that live off of chemical gradients could be considered one of the earliest deterministic steps in the chain of molecular evolution that led to chemical life. Whether biogenesis is reproducible is unclear and without this MEP may not be applicable to biotic activity.

However, once we have biogenesis, can MEP be applied to photosynthesis or a given species? Surely there must be a spectrum of reproducibility between generic features that are reproduced (galaxies, stars and planets) and unique quirks that are not (tuataras, sulfur-crested cockatoos, HIV). One way to begin to determine this spectrum of reproducibility is by doing controlled experiments in evolution. Long term experiments in bacterial evolution can be used to test the reproducibility of metabolic adaptations to external stress such as temperature, pH and low food levels (Lenski 1998). In addition, if careful measurements of the entropy of the input nutrients and output waste can be made over long periods, evolution towards (or away from?) entropic maxima can be quantified.

References

Bekenstein JD (1981) Universal upper bound to entropy-to-energy ratio for bounded systems. Phys Rev D 23: 287–298.

Bennett CL et al. (2003) The Wilkinson Microwave Anisotropy Probe (WMAP) Basic Results. Astrophys J Supp Ser 148: 1–27.

Davis TM, Davies PCW, Lineweaver CH, (2003) Black hole versus cosmological horizon entropy. Classical and Quantum Gravity 20: 2753–2764. astro-ph/0305121.

Davis TM, Lineweaver CH (2003) Expanding Confusion. Pub Astron Soc Australia 21: 97–109. astro-ph/0310808.

Dawkins R (1982) The Extended Phenotype. Oxford University Press, Oxford, pp. 234–237.

de Duve C (1995) Vital Dust. Basic Books, New York.

Dewar RC (2003) Information theory explanation of the fluctuation theorem, maximum entropy production and self-organized criticality in non-equilibrium stationary states. J Phys A 36: 631. also at http://arxiv.org/abs/condsmat/0005382.

Frautschi S (1982) Entropy in an Expanding Universe. Science 217: 593–599.

Jaynes ET (1957) Information theory and statistical mechanics II. Phys Rev 108:171–190.

Lenski RE et al. (1998) Evolution of competitive fitness in experimental populations of E.coli: What makes one genotype a better competitor than another? Antonie van Leeuwenhoek 73: 35–47.

Lineweaver CH, Davis, TM (2002) Does the rapid appearance of life on Earth suggest that life is common in the Universe? Astrobiology 2/3: 293–304. astro-ph/0205014.

Lorenz RD, Lunine JI, Withers PG, McKay CP (2001) Titan, Mars and Earth: Entropy production by latitudinal heat transport. Geophys Res Lett 28, 415–418.

Lorenz R (2003) Full Steam Ahead-Probably. Science 299:837–838.

Lotka AJ (1922a) Contribution to the energetics of evolution. Proc Natl Acad Sci USA 8: 147–151.

Lotka AJ (1922b) Natural selection as a physical principle. Proc Nat Acad Sci USA 8: 151–154.

Lovelock JE (1972) Gaia: A new look at life on Earth. Oxford University Press, Oxford.

Lovelock JE (1988) Ages of Gaia. Norton:NY.

Lovelock JE, Margulis L (1974) Atmospheric homeostasis by and for the biosphere: the Gaia hypothesis. Tellus 26: 2–10.

Nealson KH, Conrad PG (1999) Life, past, present and future. Phil. Trans. Roy. Soc. Lond. B 354:1–17.

Paltridge GW (1975) Global dynamics and climate – a system of minimum entropy exchange, Q J R Meteorol Soc 101: 475–484.

Paltridge GW (1979), Climate and thermodynamic systems of maximum dissipation. Nature 279: 630–631.

Pavlov A, Kasting J, Brown L, Rages K. Freedman R (2000) Greenhouse warming by CH_4 in the atmosphere of early Earth. J Geophys Res 105:11981–11990.

Prigogine I (1980) From Being to Becoming. WH Freeman, New York.

Ulanowicz RE, Hannon BM (1987) Life and the Production of Entropy. Proc R Soc Lond B 232: 181–192.

Watson AJ, Lovelock JE (1983) Biological homeostasis of the global environment: the parable of Daisyworld. Tellus 35B: 284–289.