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

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Abstract

The Maximum Entropy Production Principle (MEPP) 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 MEPP should apply. Whether the concept of MEPP 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.

The Maximum Entropy Production Principle and Reproducibility

The Maximum Entropy Production 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 the MEPP predicts that winds and currents driven by thermal gradients will set up in a way to maximize entropy production (Paltridge 1979, Lorenz 2003).

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 don't need to describe the microstates accurately and we don't 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 don't know which one -- so the larger W is, the larger our ignorance and the larger the entropy. In recent ground-breaking work, Dewar (2003a) has provided a derivation of the Maximum Entropy Production Principle. Dewar points out that our ignorance can be applied to non-equilibrium systems (Jaynes 1957). In Dewar's derivation of the MEPP, 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 don't need equilibrium but we do

need reproducibility, and thus reproducibility becomes the key to whether the MEPP can be applied.

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 the MEPP to cosmology and biology. However, since the MEPP is limited to reproducible dissipative structures we need to identify such structures in cosmology and biology.

Cosmological Reproducibility

Let's 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. 1). Galaxies form Stars and planets condense from swirling dissipative accretion disks. again. 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 MEPP should apply to all of them.

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 structures) needs gradients to form and survive, the initial condition of any universe that contains life will be one of low entropy, not high entropy. You can't 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 (during a short period at the end of inflation called reheating) from the decay of the evenly distributed potential energy of a scalar field. '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 and clump. The gravitational potential

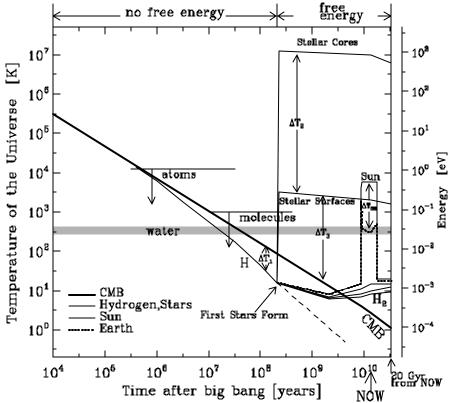


Figure 1 Reproducible aspects of the evolution of our universe. As the universe expands, its temperature (the temperature of the CMB) decreases as: $T_{CMB} \sim 1/size$. Half a million years after the big bang, the temperature of the universe falls beneath the binding energy of hydrogen. Atoms form. 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/size². 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 "?T1" above. As the hydrogen cools further to T ~ 20 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 ~ 10^7 K at their cores and ~ 10^3 - 10^4 K at their surfaces. This temperature difference is labeled '?T2' 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 '? T3'. The Sun /Earth temperature difference responsible for all life on Earth is labeled ?TSE. 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 $?T_{SF}$: 6000 K / 300 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 ~ 0.2 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 ~ 1 eV from each solar photon.

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.

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 and whether the expansion of the universe produces entropy.

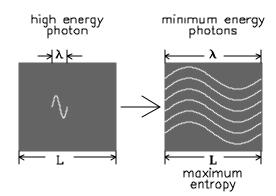
It is difficult to talk about the total entropy in the universe without knowing how big the universe is. So we talk about the entropy in a representative sample of the universe. Typically we put an imaginary sphere around a few thousand galaxies and consider the entropy in this sphere. As the universe 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 ~ 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 ~ R^3 . And since the temperature of the microwave background goes down as the universe expands: T ~ 1/R, we have the result that the entropy of a given comoving volume of space S ~ $R^3 * R^3$ = 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 produces no entropy, what does? Any region of the universe can be considered as an isolated cosmic box. The reason 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 (? T_2 in Fig. 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 $S \sim kN$ 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 ~ 1 % of the number of CMB photons. The entropy of the universe would increase by only 1%.

Figure 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 > 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 $E_{min} = hc / ?_{max} = hc / L$. Thus, we have $S_{max} = k E L / hc$, and the result that the maximum entropy of the universe is proportional to the increasing size of the universe: $S_{max}(t) \sim L(t)$ (see Fig. 3 for limits on this size).

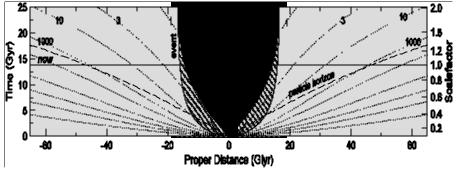


Figure 3 The maximum size L of the system in Fig. 2 is the cosmic event horizon shown here. As the universe expands the only part of it we can see is along our tear-dropped shaped past light cone. As the universe gets older, our past light cone asymptotically approaches the event horizon. Our worldline 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 ?, the universe has an event horizon whose largest radius will be ~ 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: $?_{max} \sim 36$ billion light years. The cosmic event horizon imposes a maximum physical size to the observable universe and therefore a maximum wavelength of light ?max. Therefore, since $S_{max}(t) \sim L(t) => L_{max}$, S_{max} approaches a constant. The temperature of the universe approaches $T_{?}$ and a heat death for the universe is possible ($S_{universe} ==> S_{max}$). In such a situation the energy within the event horizon goes down and one would expect $S_{\!nax}$ 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 2003).

Return of the Heat Death

Before the discovery that 3/4 of the energy density of the universe was vacuum energy (? $_{?} \sim 0.73$), 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 a cosmological constant creates a cosmological event horizon 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:

 $T_{?} = 1 / 2? ?^{1/2}$.

This is the minimum temperature that our universe will ever have if the cosmological constant is a true constant. Current values of ? yield $T_2 \sim 10^{-30}$ 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.

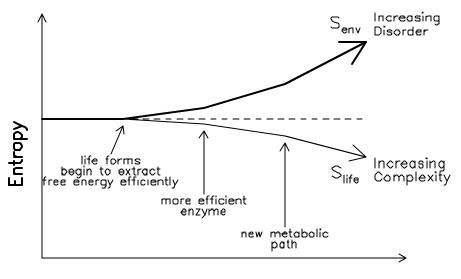
To summarize our cosmological considerations: Galaxies, stars and planets are reproducible structures and should be describable with the MEPP. The expansion of the universe, by itself produces no entropy. Stars currently are the largest producers of entropy in the universe but all the stars in the universe 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.

Biological Reproducibility

Does life increase the total entropy growth over what it would be without life?

Much evidence supports the idea shown in Fig. 4 that life increases the rate of entropy production. For example, forests are cooler than deserts at the same latitude and thus produce more entropy. The decreasing ' S_{life} ' of Fig. 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.

"If two systems receive the same quantity of energy at the same entropy, that system which extracts **h**e 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." (Ulanowicz and Hannon 1987). Thus, the evolution of more efficient metabolisms is equivalent to the evolution of larger entropy production.



time

Figure 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: $dS = dS_{life} + dS_{env} \ge 0$. 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 its metabolic paths become more efficient at extracting available free energy and this is represented by the changing slopes.

Figure 4 represents biological dissipative structures increasing net entropy ($dS = dS_{sys} + dS_{env} \ge 0$). We assumed a constant baseline of abiotic entropy (horizontal dashed line). More realistically we need to include the abiotic entropy production of weather on a planet (Fig. 5).

In Lovelock's Daisy World (Lovelock 1988) daisy albedo regulates planetary temperature. The fact that the Sun's luminosity is increasing puts the focus on temperature reduction (= entropy increase). However, a symmetry is assumed: that it is just as easy to increase the temperature as decrease it. Thus the assumption is made that entropy decrease is just as likely as entropy increase. Such feedback mechanisms between dissipative systems are candidates for a violation of the MEPP 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. 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 invoke biotic methanogenesis to warm the early Earth and reduce its entropy production (Pavlov etal 2000).

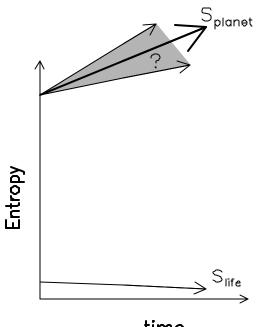


Figure 5 Entropy of a planet (and life on that planet) as a function of time. The small decreasing entropy of life is negligible compared to the entropy and entropy production of the planet. If feedback mechanisms regulate the temperature of the planet, life can either increase or decrease the entropy production of the planet (grey region around S_{planet}).

time

Applying the maximum entropy principle to biological evolution

One problem with applying the MEPP 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. 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 the MEPP prescribes stable maxima for non-living dissipative structures and transient local maxima for life.

In the general debate surrounding Lovelock's Gaia hypothesis 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 the maximum entropy principle, can be successfully used to describe evolution, then considering the biosphere as an evolving life form seems more appropriate. Competing life forms can be compared to the competing micropaths in Dewar's derivation of the MEPP. As Dewar has pointed out, these micropaths do not have to be realized for the end macrostate to obey the MEP. This contrasts with Dawkins' view that the competitors need to be present for selection to be meaningful.

Does the MEPP 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 MEPP have anything to say on this issue?

Among the structures in the universe, far from equilibrium dissipative structures (Prigogine 1980) are ubiquitous and inhabit regions of thermal and chemical gradients. Stars, convection cells, whirlpools, and hurricanes are common. The MEPP should apply to these reproducible macrostates. The formation of autocatalytic 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 the MEPP can not be applied.

However, once we have biogenesis, can the MEPP 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, 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.

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