

Self-Assembling Universes Maximize Novelty

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Abstract:

The Universe appears to be inherently unpredictable, not just for fundamental reasons from the limits of mathematical proof, or the consequences of quantum mechanics, but also due to how complex systems express or develop new rules at higher levels which emerge independently of their lower levels. However, most of these complex systems are still simple, and have few constraints which places limits on the nature of the unpredictability of the dynamics shown by these systems. Living systems are not only able to exhibit more unpredictable behaviors, but these are intrinsically more novel than the unpredictable behaviors associated with the abiotic universe. In this essay I discuss how a new theory I have been developing, assembly theory, can be used to identify if a given object has been constructed or not by exploring the constraints required for the object to form from undirected or random processes. I try to explain that the more assembled a given a system is, the more of the possible state space is accessible, and hence how both unpredictable and capable of generating novelty the system is. Finally, I argue that living systems are also intrinsically unpredictable in terms of their ability to express novelty and outline a scale of assembly which might provide a way to distinguish living systems from non-living systems.

Introduction

In the time of the Newtonian Universe everything was predictable and our notion of ‘free will’, complexity, and the richness of reality could be mechanically described if enough information was known to an almost infinite precision. The era has ended and today most, if not all, physicists would agree that the Universe appears to be inherently unpredictable. In this essay I will argue that there is something additional missing from this viewpoint. Whilst I agree there are many reasons why the universe is intrinsically unpredictable, the nature of that unpredictability is unremarkable or boring where the universe involved is dead i.e. does not contain living systems. Living systems appear to introduce a different type of unpredictability and novelty that is absent in non-living systems. An objective of this essay is that explain how it might be possible to quantify this unpredictability with experimental measurements, and hence distinguish between objects and processes that are the product of life rather abiotic processes.

Before exploring the idea of the uniqueness in living systems we must digress to discuss how we explain disorder using the concept of Entropy. Clausius took the term ‘entropy’ from the Greek word for evolution or transformation. From a chemical point of view the entropy change of a system is defined by the reversible heat addition to the system divided by its absolute temperature but Boltzmann developed a statistical mechanical explanation reducing macroscopic states to microscopic states. This means that statistical mechanics explains a macrostate by microstates i.e. the observable macrostate is realized by many microstates. This means that for the second law to hold, the universe must have started in a very low entropy state if we are going to assume an arrow of time. However, I find the use of entropy unsatisfactory since it explains how disorder develops and the way the course graining is done means that the context is often lost. Perhaps a new approach that can take into account the history or literally how the universe remembers

enough information to build the object, without loss of context, might provide a new lens through which to see if such objects can only be produced by functional selection that occurs in living systems.

In the thought experiment known as the “infinite monkey theorem”, an infinite number of monkeys, each having a typewriter, produce strings of text by hitting keys at random [1]. Given infinite resources, it can be deduced that the monkeys will produce all possible strings, including the complete works of Shakespeare. However, when constrained to the bounds of the physical universe, the likelihood that any particular text is produced by a finite number of monkeys drops rapidly with the length of the text [2]. This can also be extended to physical objects like airplanes and the “junkyard tornado”. Fred Hoyle speculated that the probability of abiogenesis is like that of a tornado sweeping through a junkyard and assembling a Boeing 747 jumbo jet airplane [3]. Given infinite resources, it can be deduced that the tornado will produce all possible configurations, including every possible plane that could be designed and built by Boeing. Even if we were to convert nearly all matter in the universe to object constructing monkeys, and give them the age of the universe in which to work, the probability that any monkey would construct any sufficiently complex physical object is negligible [4], in fact I would go further to say the probability is precisely zero as the argument is not well posed. As it stands, the thought experiment is an entropic argument – the number of possible arrangements of the objects of a given composition increases exponentially with the object size. Indeed, if the number of possible play-sized strings is sufficiently large, it would be practically impossible to produce a predetermined Shakespearean string without the author. This argument implies information external to the object itself is necessary to construct an object if it is of sufficiently high complexity [5]: in biology the requisite information partly comes from DNA, the sequence of which has been acquired through countless cycles of evolution and the cost of these cycles in terms of time and resource is significant. Although Shakespeare’s works are – in the absence of an appropriate constructor [6] (an author) - as likely to be produced as any other string of the same length, our knowledge of English, and Shakespeare in particular, allows us to partition the set of possible strings into those that have meaning, and those that do not, and to assess the very low probability that we would be presented with a random long string that has meaning.

Information and Complexity

Biological systems have access to a lot of information - genetically, epigenetically, morphologically, and metabolically - and the acquisition of that information occurs via evolutionary selection over successive cycles of replication and propagation [7]. One way to look at such systems is by comparing the self-dissimilarity between different classes of complex system, allowing a model free comparison [8]. However, it has also been suggested that much of this information is effectively encrypted, with the heritable information being encoded with random keys from the environment [9]. As such, these random keys are recorded as frozen accidents and increase the operative information content, as well as help direct the system during the process of evolution, producing objects that can construct other objects [10]. This is significant since one important characteristic of objects produced autonomously by machinery (such as life), which itself is instructed in some way, is their relative complexity as compared to objects that require no information for their assembly beyond what chemistry and physics alone can provide. This means that for complex objects there is ‘object-assembly’ information that is generated by an evolutionary system and is not just the product of laws of physics and chemistry alone. Biological systems are the only known source of agency in the universe [11], and it has been suggested that new physical laws are needed to understand the phenomenon of life [12]. The challenge is how to explore the complexity of objects generated by evolutionary systems without a priori having a model of the system.

In computer science Kolmogorov complexity [13] is one of the core complexity concepts, being the length of the shortest program (in a given Turing-complete language) that can produce a given output. Closely related is the notion of logical depth [14]. Given the shortest program that generates a given object, its logical depth is the computational time necessary to generate it from that program. A more involved definition is usually given, allowing the consideration of programs which are slightly longer than the shortest possible, but significantly faster to run, with the logical depth at a level of significance n considering all programs no more than n bits longer than the shortest, but we do not discuss this in detail here. In Bennett's this demonstrates an attempt to quantify the intuitive difference, in both physical and abstract cases, between "trivial" objects and those with a "nontrivial causal history". The same paper further considers its machine-independence and relation to self-organization. Attempts have been made to apply logical depth and algorithmic complexity (of which Kolmogorov complexity is the most commonly used version) to biological systems and subsystems. Collier [15] proposes the use of logical depth as a general definition of "organization" that can be applied to them. Other factors such as dynamic processes are considered relevant.

Algorithmic information theory has been summarized [16] as, "an attempt to apply information-theoretic and probabilistic ideas to recursive function theory." It encompasses several core ideas in the study of complexity, such as the minimum number of bits required to specify an algorithm. It also considers probabilistic approaches to solutions. Coming at the topic from a cryptographic angle, one paper considers the minimal program and input necessary to generate a pseudo-random string, in the style of Kolmogorov complexity. On the other hand, "effective complexity" is defined as a measure of the information content of the regularities of an object, originally introduced by Gell-Mann and Lloyd to avoid some of the perceived disadvantages of Kolmogorov complexity. It has been refined [17] with a precise definition in the language of algorithmic information theory, and analyze it further – for example, by comparing it to other measures. It also has a strong relation with logical depth. "If the effective complexity of a string exceeds a certain explicit threshold then that string must have astronomically large depth; otherwise, the depth can be arbitrarily small." Other attempts have been made to fully embody information theory concepts in physical processes, such as by starting from a physical definition of "meaningful information" [18].

A New Approach

A few years ago, I developed some ideas that would lay the foundations of a new theoretical approach to agnostically quantify the amount of historical information or pathway assembly information contained within an object. I reasoned this could be achieved by considering how the object can be deconstructed into its irreducible parts, and then evaluating the minimum number of steps necessary to reconstruct the object along any pathway. As a chemist, I naively thought about taking a molecule and cutting it up into pieces such that I could easily use the shortest route to reassemble the molecule. In thinking about this approach, I realized the analysis of pathway assembly is done by the recursive deconstruction of a given object using shortest paths, and this can be used to evaluate the effective pathway assembly index for that object [19]. To take this forward I developed assembly theory within my team and collaborators [20]. In developing pathway assembly, I was motivated to create an intrinsic measure of an object forming through random processes, where the only knowledge required of the system is the basic building blocks and the permitted ways of joining structures together. This allows determining when an extrinsic agent or evolutionary system is necessary to construct the object, permitting the search for complexity in the abstract, without any specific ideas of what is looked for, thus removing the requirement for an external imposition of meaning, see Figure 1. I also imagined, if such systems could be explored at the molecular level, it should be theoretically possible to quantify the degree of assembly by using a spectroscopic technique. This because state of the art analytical

techniques such as high resolution nuclear magnetic resonance and infra-red spectroscopy, as well as mass spectrometry could all be used to read out how many unique parts a molecule has.

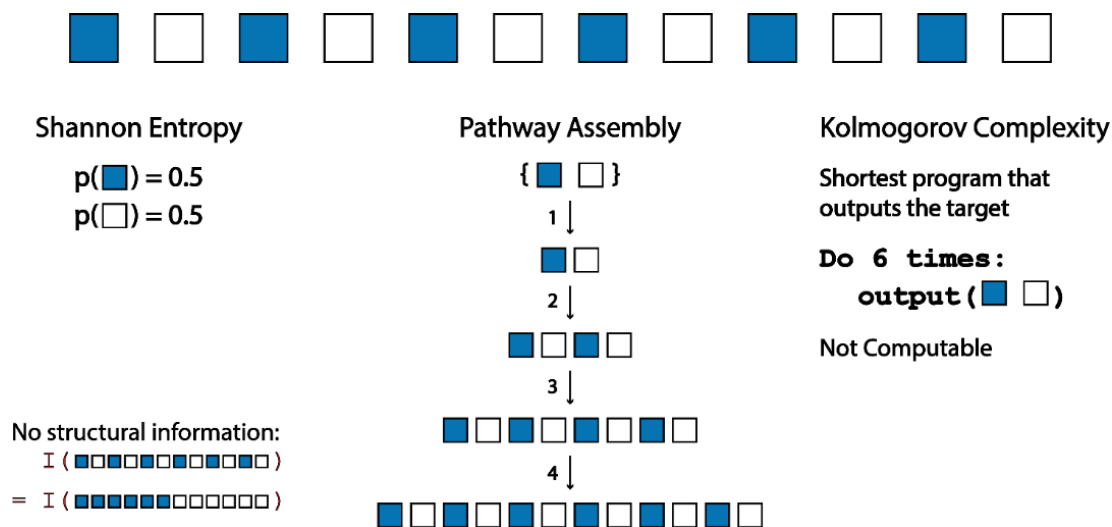


Figure 1: The Pathway Assembly process (center) [19] is compared to implementations of Shannon Entropy [21] (left) and Kolmogorov Complexity [13] (right) for blue and white blocks. The Pathway Assembly process leads to a measure of structural complexity that accounts for the structure of the object and how it could have been constructed, which is in all cases computable and unambiguous.

The development of the Pathway Assembly index (PA) was motivated by the desire to define a biological threshold, such that any object found in abundance with PA above the threshold would have required the intervention of one or more biological processes to form [20]. The Pathway Assembly index (PA) of an object is the length of the shortest pathway to construct the object starting from its basic building blocks. It should be noted that this approach is entirely classical, allowing quantifying pathways through assembly space probabilistically as a way to understand what life does. We construct the object using a sequence of joining operations, where at each step any structures already created are available for use in subsequent steps, see Figure 2. The shortest pathway approach is in some ways analogous to Kolmogorov complexity, which in the case of strings is the shortest computer program that can output a given string. However, Pathway Assembly differs in that we only allow joining operations as defined in our model. This restriction is intended to allow the Pathway Assembly process to mimic the natural construction of objects through random processes, and it also importantly allows the PA of an object to be computable for all finite objects.

Given a system where objects interact randomly and with equal probability, it is intuitively clear that the likelihood of an object being formed in n steps decreases rapidly with n . However, it is also true that a highly contrived set of biases could guarantee the formation of any object. For example, this could occur if we were to model the system such that any interactions contributing to the formation of the object were certain to be successful, while other interactions were prohibited. For complex objects, such a serendipitous set of biases would seem unlikely in the absence of external information about the end products, but physical systems generally do have biases in their interactions, and we can explore how these affect the likelihood of formation of objects. However, we expect for any perceived “construction processes” that requires a large

enough set of highly contrived biases, we can deduce that external information is required in the form of a “machine” that is doing the constructing.

Technological processes are bootstrapped to biological ones, and hence, by extension, production of technosignatures involves processes that necessarily have a biological origin. Examples of biosignatures and technosignatures include chemical products produced by the action of complex molecular systems such as networks of enzymes [22], and also objects whose creation involved any biological organisms such as technological artefacts, complex chemicals made in the laboratory [23], and the complete works of Shakespeare. Finding the object in some abundance, or a single object with a large number of complex, but precisely repeating features, is required in order to distinguish single random occurrences from deliberately generated objects. For example, a system which produces long random strings will generate many that have high PA, but not in abundance. Finding the same long string more than once will tell us that there is a bias in the system towards creating that string, thus searching for signatures of life should involve looking for objects with high PA found in relatively high abundance.

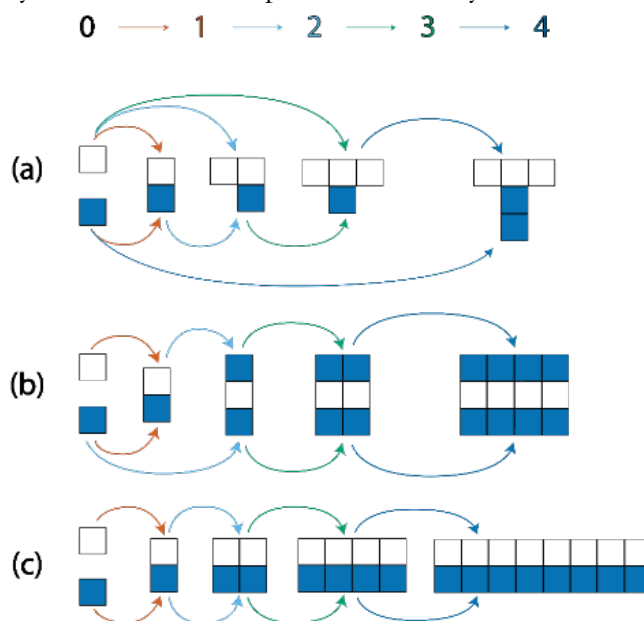


Figure 2: The concept of pathway assembly is shown here. Each of the final structures can be created from white and blue basic objects in four joining operations, giving a Pathway Assembly Index of 4. Pathway (a) shows the creation of a structure that can only be formed in four steps by adding one basic object at a time, while pathway (c) represents the maximum increase in size per step, by combining the largest object in the pathway with itself at each stage. Pathway (b) is an intermediate case.

Formally, it is possible to explore the foundations of Pathway Assembly, as well as some of its properties and variants. Also, by describing how Pathway Assembly can be incorporated into a new information measure, Pathway Information, and how this can help identify objects, above a threshold, that must have been produced by living systems. The Pathway Assembly process is formally defined in the context of an Assembly Space, which comprises an acyclic quiver Γ (a quiver being a directed graph that allows multiple edges between pairs of nodes and has no directed cycles), where the vertices in the quiver are objects in the space, along with an edge labelling map ϕ which associates each edge with a vertex in the quiver. The quiver is associated with a reachability relationship \leq where for vertices a, b in Γ , $a \leq b$ if there is a path from a to b , in other words it is possible reach b starting at a by following a sequence of edges along their respective directions. If for an edge e from object x to object z , $\phi(e)=y$, then this can be thought of as z being constructed through the combination of x and y . We also require that the symmetric operation exists within the space, i.e. there is an edge g from y to z such that $\phi(g)=x$. We define an assembly subspace Δ on an assembly space Γ to be an assembly space that contains a subset of the objects in Γ , maintaining all the relationships between them. An assembly subspace is said to be rooted if it contains a nonempty subset of the basic objects. This is an important distinction in the definition of the Assembly Index below, as it allows us to define the shortest construction pathway for objects using a consistent set of basic objects. We define the basis of an Assembly Space Γ as the set of minimal vertices in the space with regard to \leq , and refer to those vertices as basic objects, basic vertices, or basic elements. We define an assembly map as a map from

one assembly space Γ to another Δ that maintains the relationship between objects, but may map multiple objects in Γ to the same object in Δ . One such map that is generally applicable is the mapping of each object to its size, see Figure 3. Assembly maps can be useful for finding a lower bound to the assembly index, by mapping to a system that may be more computationally tractable to work in than the original system of interest.

We define the cardinality and augmented cardinality as the number of objects in the assembly space, where the augmented cardinality excludes the basic objects (defined separately, as this measure is used in the assembly index). We then define an assembly pathway and the assembly index. An assembly pathway is a set of all the objects in an assembly space Γ in some order that respects the reachability relationship \leq , i.e. a topological order. If we take all the rooted assembly subspaces of Γ that contain some object x , we then define the assembly index as the augmented cardinality of the smallest rooted assembly subspace that contains x . The subspace must be rooted, as otherwise a subspace containing only x would meet this criterion. We use the augmented cardinality of this subspace, as defined above, as defining the assembly index without including basic objects in accord with the physical interpretations that motivated this measure; however, the cardinality could instead be used if desired, and the difference in the measures for any structures with shared basic objects would be constant. The assembly index then represents the minimum number of joining operations required to construct object x , as illustrated in Figure 2.

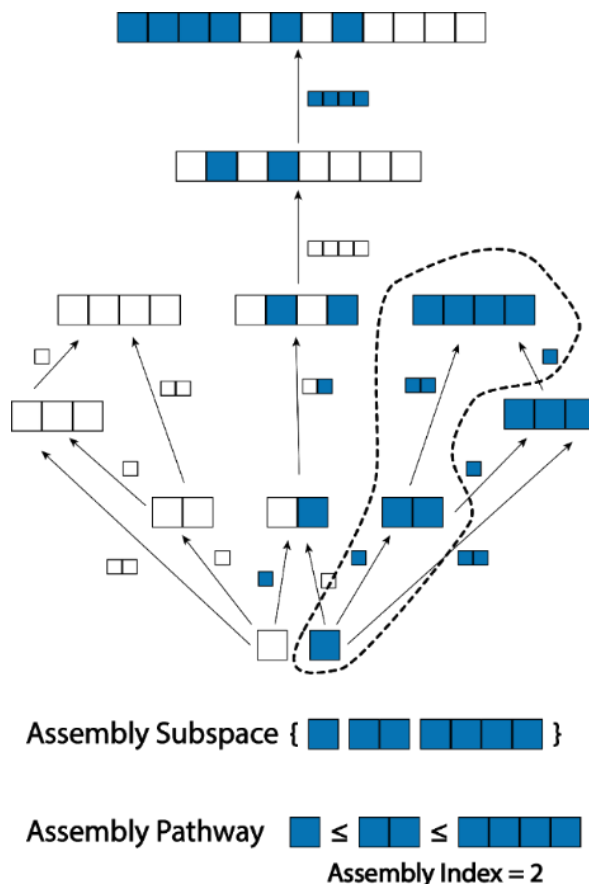


Figure 3: An assembly space comprised of objects formed by joining together white and blue blocks. Some of the morphisms have been omitted for clarity. The dotted region is an assembly subspace, and topological ordering of the objects in the subspace represents a minimal assembly pathway for any subspace containing the sequence of four blue boxes.

When mapping from assembly space Γ to assembly space Δ through an assembly map f , the assembly index of a mapped object in Δ acts as a lower bound for the assembly index of the original object in Γ . This can allow us, for example, to map an assembly space to another in which finding the assembly index is less computationally intensive in order to calculate a useful lower bound. The assembly index of an object in any rooted assembly subspace of Γ is an upper bound for the assembly index of the object in Γ . A split-branched space is an assembly space Γ where for each pair of objects x, y in Γ , $x \leq y$ or $y \leq x$ whenever $\vee(x \downarrow) \cap \vee(y \downarrow) \neq \emptyset$. This means that, other than basic objects, when combining two different objects neither of them can have an assembly pathway that uses objects created in the construction of the other. They may use objects that are considered identical (e.g. the same string) but these are separate objects within the space. Since we can define an assembly map that maps these identical objects to a new space where they map to the same object, the split-branched assembly index for a system is an upper bound for the assembly index on that system.

A Scale of Assembly, Unpredictability, and Novelty

Using the assembly theory approach it is possible to calculate the number of discrete steps required to build a given object, from a set of objects that use common building blocks, for example organic molecules, and then explore the probability of the distribution of possible objects as a function of the number of steps, frequency, and resources available. This can be illustrated simple with the space of integers under addition to explore these assembly maps, where an addition chain for an integer is a sequence of integers, starting with 1, with each integer in the sequence being the sum of two previous integers, see Figure 4 [24]. A minimal addition chain for an integer is the shortest addition chain that terminates in that integer, and the size of that addition chain is equivalent to the pathway assembly index of the integer (after subtracting 1 to account for the single basic object). The objects in this space can be considered as abstract integers, or as representing the size of objects in some other assembly space. It is possible to model the assembly process as a weighted decision tree where at each level there is a choice of objects that can be formed. The number of choices at each level of the tree is constrained by the number of integers that have the assembly index associated with that level.

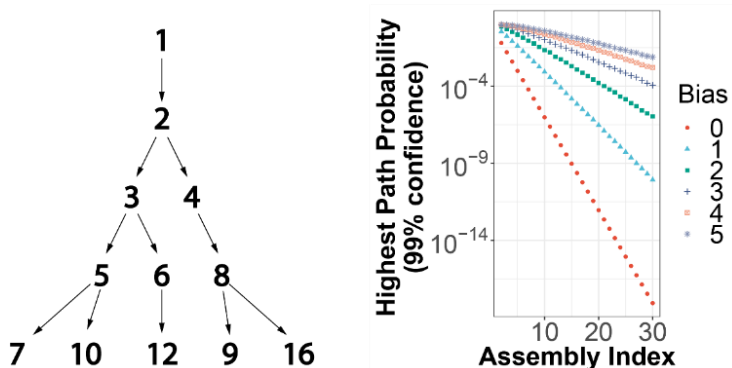


Figure 4: Left – Minimal addition chains modelled as a decision tree. Right – probability of the most likely pathway at different levels of bias. Data from all minimal addition chain lengths for integers up to 100,000 was used.

These probabilities will reduce further when considering greater number of choices, such as in situations of higher dimensionality, like strings, grid structures, and graphs. In the maximum bias case explored here, where $h=5$, the choices with $x=5$ will be 10,000 times more likely than those with $x=1$. This argument demonstrates that using a pathway assembly model will result in a threshold above which it is unlikely that any specific object would be found, with the threshold depending on the system of objects and joining operations, and the physical limits of the inherent biases present in the process. Even in a significantly biased system, such a threshold will exist, and any objects found in abundance with the assembly number being above the threshold will require some process inducing specificity outside of the random (bias) model to form. The more constructed the object, it is possible to think of extremely intricate architectures that are so surprising or unprecedented that these objects can be considered to be novel. Novelty is a relative term but in general something is novel if the configuration or representation is so unusual compared to what is already known, that it gives an entirely new set of transformations not before known (within the known universe). Living systems generate novelty all the time via the process of Darwinian evolution and hence I'm insisting that this term is at least superficially introduced here since it appears to be important in distinguishing the purely physical law-governed universe without living systems, from a universe capable of open ended evolution searching for ever more non-trivial trajectories in a state-space.

Conclusions

In this essay I've described how Assembly Theory can be used to differentiate between objects, patterns and systems that are produced in the universe by undirected processes vs. those produced by evolutionary systems, and my team have built on our initial work[19] by establishing a robust mathematical formalism

with our collaborators [20]. By establishing the limits of Assembly Theory, and how it might be experimentally measured for a given set of objects, it will be possible to define a scale that connects the degree of history needed or memory required as the system that produces it becomes more life-like. Ultimately it might be possible to rigorously establish a threshold above which extrinsic information from a biological source would have been required to create an observable abundance of an object. This is because the object has too many features to have formed in abundance without some constraints on the degrees of freedom. Finally, I want to argue that the degree of assembly is not only a measure of the unpredictability or novelty associated with the states that produced that system, I want to go further and say that in the extreme the more unpredictable or novel the system is, the more life like it is. I think this is a very important outcome not just theoretically, but because I think that objects, with assembly numbers above a certain threshold, can be uniquely assigned as have been produced by a biological process. In other words, it can be used to detect biological influence even when we don't know what we are looking for. I'm excited by this approach since it will yield an experimental measure that will allow the degree of assembly that a given object has had in terms of a supporting infrastructure to build the object. Put another way the theory of object assembly allows us to place a degree of surprise or novelty associated with finding that object in a given environment.

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