

The Physics of Causation

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Abstract

Assembly theory (AT) introduces a concept of causation as a material property, constitutive of a metrology of evolution and selection. The physical scale for causation is quantified with the assembly index, defined as the minimum number of steps necessary for a distinguishable object to exist, where steps are assembled recursively. Observing countable copies of high assembly index objects indicates that a mechanism to produce them is persistent, such that the object's environment builds a memory that traps causation within a contingent chain. Copy number and assembly index underlie the standardized metrology for detecting causation (assembly index), and evidence of contingency (copy number). Together, these allow the precise definition of a selective threshold in assembly space, understood as the set of all causal possibilities. This threshold demarcates life (and its derivative agential, intelligent and technological forms) as structures with persistent copies beyond the threshold. In introducing a fundamental concept of material causation to explain and measure life, AT represents a departure from prior theories of causation, such as interventional ones, which have so far proven incompatible with fundamental physics. We discuss how AT's concept of causation provides the foundation for a theory of physics where novelty, contingency and the potential for open-endedness are fundamental, and determinism is emergent along assembled lineages.

Introduction

Beyond a certain complexity threshold, the spontaneous formation of objects becomes vanishingly improbable, if not impossible. The chance of spontaneous formation for even moderately complex objects is small enough that this has never been observed to happen. While spontaneous generation was ruled out as a plausible explanation for microbes over a century ago¹, fluctuation into existence of arbitrarily complex objects persists as something allowed by current physics, introducing theoretical pathologies (e.g., Boltzmann brains, and requiring fine-tuning)^{2,3}. A more parsimonious explanation is that complex objects must be caused to exist, but this is incompatible with current physics, which has no concept of 'cause'.

Prior to the 1800s, life's origin was thought to be spontaneous. A prominent example was in how broth, even after boiling, if left in the open would sprout micro-organisms⁴. Careful experimental control of environmental and other causal influences has repeatedly demonstrated the process of generating microbes is not spontaneous; for example, experiments of sterilized broth insulated from contamination exhibit zero growth of *de novo* complex, biological forms¹. Likewise, many structures human chemists might envisage are so complex, they will *never* be observed to emerge spontaneously within any span of finite time and finite resource. This is because the causation mediating their formation does not itself exist.

The observable universe contains $\sim 10^{80}$ atoms. Taxol, a secondary metabolite with molecular formula $C_{47}H_{51}N_1O_{14}$, shown in **Figure 1**, is one among an estimated $\sim 10^{100}$ possible molecules⁵ with molecular weight < 1000 Amu. Not all $\sim 10^{100}$ possibilities will ever exist. There are no instantiated mechanisms (catalysts) for making the majority, and there are not enough atoms in the entire universe to make them all in any case. For Taxol, the chance of producing it spontaneously, by joining 47 carbon, 51 hydrogen, 1 nitrogen and 14 oxygen atoms in the precise 3D arrangement of Taxol,

is far smaller than 1 in 10^{23} (less than one molecule per mole of sample) with both the desired formula and 3D conformation. The exact, spontaneous probability cannot be defined: the size of chemical space is vast and not computable, and it cannot ever be fully explored to assign probabilities to all possible structures within it.

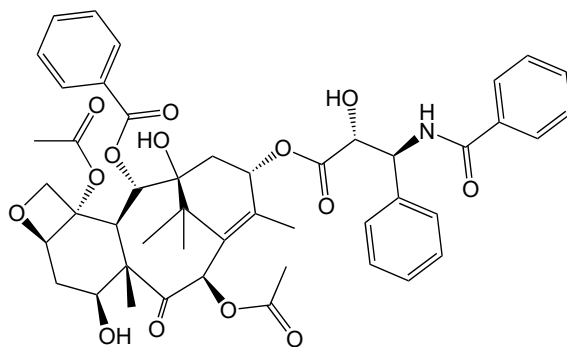


Figure 1. Taxol's chemical structure with formula $C_{47}H_{51}NO_{14}$. The molecular weight is 853.91 g/mol, and with 11 chiral centres there are 2^{11} or 2048 possible stereoisomers, which likely drastically underestimates the number of molecular structures with this same molecular formula.

Using $\sim 10^{100}$ as a lower bound on the number of possibilities in the space indicates the expected spontaneous molar concentration is so low that human chemists should never observe Taxol, if it formed solely via spontaneous generation, and an ergodic sampling of chemical space. In bark extracts from the Pacific Yew tree, Taxol is abundant with a concentration $\sim 20 \text{ ug g}^{-1}$ of bark (*ca.* 10^{16} molecules g^{-1}). Copies of Taxol are reliably synthesized as a secondary metabolite within Pacific Yew bark, itself the product of billions of years of evolution constructing a specific organism that can itself construct Taxol. For Taxol, both the biosynthetic, and also a semi and fully synthetic route for its synthesis are known⁶⁻⁸.

How could we know Taxol must be the product of an evolutionary lineage, if we did not know anything about *how* it was made? This is one in the same as Paley's famous question about how one might determine design in a watch⁹, but here applied to molecules as more tractable physical objects of study.

Paley intended his watch argument to be in favour of a theological explanation for design in nature. An alternative view is that the appearance of design, without a designer, can be explained naturalistically via scientific methods. Darwin's "struggle for existence" introduced natural selection as an explanation for some features of organic design¹⁰, via the mechanism of survival of the fittest. But natural selection is a passive filter, culling already-created forms to leave only the most persistent (adapted).

A focus only on existing forms misses most of the causal work selection does. For example, it does not account for how new forms arise, and why evolution has discovered so many new, often complex forms so rapidly¹¹. Existing theories do not explain why new lineages emerge, or the major transitions that branch them into radically different forms, including transitions in substrate³. Two significant transitions are the emergence of biological lineages from geochemistry¹², and the emergence of technological lineages from biology¹³, where both biological and technological lineages also have many branches¹⁴. As Krakauer has pointed out, explaining design encompasses many of the goals in the emergence of complexity science in the last century (see early work by Simon¹⁵), which is unified across its many applications as field studying designed objects¹⁶. These include those of biological, technological or even alien (if these exist) origin.

Assembly theory (AT) introduces a standardizable, physical scale for constructed complexity by elevating causal possibilities to the status of a physical space, the assembly space¹⁷, which can be metrologically explored¹⁸. Within this space, objects are defined by their assembly index, the minimum causal steps necessary to construct them. Assembly space makes it possible to quantify a threshold, below which objects form spontaneously, and above which specific selective circumstances, the kind known only to arise through extant evolutionary or intelligent lineages, are necessary for an object to exist and be measured. Thus, AT provides a theoretical framework to

allow experimental tests of whether objects like Taxol are objectively ones that *cannot* form spontaneously. AT's principles can be tested as a general theory of causation in substrates beyond molecules.

Here, to introduce the core concepts, we demonstrate the existence of a well-defined upper limit to what is abiotically possible relying only on a few, reasonable assumptions. We start via a theoretical proof of an abiotic upper bound in assembly space and its relationship to experimental tests. We use this as a segue into explaining AT's implications as a theory of physics, where causation is a definable and measurable property.

Assembly Threshold Demarcating Life

In AT, each distinguishable *object*, o_i , is defined as a physical entity that is (1) countable, (2) finite, and (3) can be disassembled (or assembled) by a finite sequence of recursive steps (see Sharma et al.¹⁷). Thought experiments on the realizability of chemical space suggest the existence of objects cannot be taken as given *a priori*, because we do not observe all possible objects (and never will). In AT, we assume as a principle of physics that causation is necessary to the existence of objects. AT starts from quantification of assembly index, a_i , specific to each distinguishable object type, i , and defined as the minimum number of causal steps necessary for that object to exist, where steps are built recursively. Recursive construction of objects defines the assembly space, delineating the set of all possible causal structures. Here causation emerges in the application of physical constraints that must be present in the object's environment; an example is how catalysis can direct the formation of a chemical bond to make a specific molecular object.

Observing countable many copies, n_i , of an object indicates a causal mechanism is persistent to produce them reliably, which must be run from an extant memory that

applies constraints in the assembly space. That is, any object persisting in environments for timescales longer than its natural half-life (timescale to decay), implies the object is constructed, and therefore can be constructed again¹⁹. A mechanism was selected that itself persists in the environment, which allows its reproduction (sometimes referred to in the abstract as a constructor, see e.g. von Neumann²⁰ or Deutsch²¹). This is nuanced. For example, a molecule's half-life is controlled by its environment. If the environment includes conditions causing the molecule to react with other things (e.g., oxidation, reduction on earth), this can cause the molecule to decompose over time. All organic matter will eventually decay to CO₂ and H₂O because these are the thermodynamically most stable products²². Yet, some molecular structures, like ribosomes²³, have persisted on Earth for billions of years. Deeper memory leads to contingency and allows the production of copies of more intricate objects, that is those with larger assembly indices.

Together copy number and assembly index allow quantifying a threshold in assembly space, below which objects might form spontaneously, and above which specific selective circumstances, the kind known only to persist in extant evolutionary or intelligent lineages, are necessary for an object to exist and be measured.

Here, we formalize our central argument. We consider two classes of objects elucidated by the example of Taxol: some objects are *spontaneous* because they can form in abundance when conditions allow, and other objects are *selected* because they require very specific circumstances for their formation against a combinatorially explosive set of possibilities. Selected objects must form along a *lineage* or causal chain specific to their formation. A key conjecture of AT is this division is not only a feature of the processes making these objects, but of the objects themselves.

Our formal argument uses a very simplified mathematical example. Although simple, it demonstrates key principles of AT as a constructivist theory of physics, where no

sufficiently high assembly object can exist in the absence of a selective mechanism for its causal construction.

Assume it takes a causal steps to construct an object (a is in assembly time, see¹⁷). Here, a causal step is defined minimally, in the joining of two structures to make a new one. In a combinatorial, recursively constructable space, the number of possible objects formed in successions of such events will grow super exponentially. We assume a branching factor, b , to parameterize this growth, which is substrate specific.

We classify indistinguishable but countable objects by type, i , where types are defined based on their distinguishability, such that the number of copies, n_i of a given type corresponds to the countable number of objects of that type, up to limits of measurement. The branching factor, b_i , for a given object type, i , is then size of the set of other structures that can be formed in one recursive causal step, using only products of preceding causal joins along a causal chain. We simplify to a global b , uniform across all structures for what follows, to allow us to illustrate our key points more straightforwardly. We expect our models presented to drastically underestimate the size of the assembly space: in physical samples we expect b to be object-dependent and increase with assembly index (e.g., branching adopts a form that is object-specific and scales with assembly index, e.g., of the form $b_i(a_i)$) leading to much more explosive combinatorial growth in the number of possibilities in real materials.

Recursion is a necessary axiom for a physics that does not allow spontaneous generation of arbitrarily complex objects: this is because, in the absence of spontaneous existence, the only way to make new objects is to use preceding structures in a causal chain. This also implicates microphysical causation as necessary to the physics we aim to describe. The exponential, combinatorial explosion of the space of possibilities with each step means there will always be a finite threshold for the causal depth of what objects can exist.

Assembly Threshold Theorem: A recursive causal threshold exists for all finite, combinatorial physical systems. Let N_T be the total number of countable objects in a sample, b the substrate-dependent branching factor (here taken globally for simplicity), and M the instrument resolution defining the minimum number of copies necessary to register measurement of an object. We denote the threshold defining the maximum assembly index of an object that can be measured in multiple copies in the absence of selection as a_M . This is bounded by:

(1)

$$a_M = 1 + \frac{\ln [M] - \ln \left[\left(1 - \frac{1}{b}\right) N_T + \frac{1}{b} \right]}{\ln \left[\frac{1}{b} \right]}$$

Proof: For an object to exist and be measured at least M copies must form. Assuming there exists a total number, N_T of objects of any kind, the expected number of countable objects, $\langle n(a) \rangle$, requiring a steps for their formation is:

(2)

$$\langle n(a) \rangle = \frac{\left(\frac{1}{b}\right)^a}{\sum_a \left(\frac{1}{b}\right)^a} N_T$$

Where b^a captures how many branches can be followed, along a causal joins, with $d(a) = \left(\frac{1}{b}\right)^a$ the number density of distinguishable object types (terminus of all branches) after a steps. The sum $\sum_a \left(\frac{1}{b}\right)^a$ provides the normalization to maintain the physical constraint that the sum over all expected copy numbers is the finite total number of objects N_T (e.g. $\sum n(a) = N_T$). We assume all branches are followed, that is, there is no selection. Since the space of objects is branching, the number density will drop off exponentially with the number of steps. For finite N_T , there will be an a where the expected number of objects is $\langle n(a) \rangle < M$, such that objects requiring more steps than a cannot be observed because the expansion of combinatorial possibilities is too vast and these can exist in copy numbers below detection limits. Setting $\langle n(a_M) \rangle = M$,

in Eq. 2, and solving for a_M gives the threshold (see Appendix B). The argument is sufficiently general to apply to any recursively constructed combinatorial space: with finite resource, all such spaces will exhaust populating possibilities in a finite number of recursive steps.

Here we introduced a forward assembly process for object construction, defining an assembly time a , as the number of discrete causal, constructive steps¹⁷. In general, assembly time (the number of steps in a forward assembly process terminating on an object) is not equivalent to assembly index. Nonetheless, Eq. 1 gives us a fundamental bound on assembly index, because the assembly time to make an object can never be less than that object's assembly index. Eq. 1 thus demonstrates, absent selection, *any* object we observe must be possible to form within a set of causal joins equal to a_M , or less, setting a fundamental causal bound on the possibility of an object to exist and be measured. Since assembly index is the minimum causation for each object, the value of a_M tells us what objects cannot form without selection, that is objects with $a_i > a_M$ cannot form abiotically. Such a bound will hold if microphysical causation is a real feature of our universe, such that all objects have a partial ordering to what can exist (e.g., an object cannot be assembled unless parts to assemble it are themselves already assembled).

By the forgoing, in a sample of N_T countable objects, those with an assembly index $a_i > a_M$, will have an expected copy number $< M$, meaning they cannot exist and be measured without some prior constraints in the branching process. That is, they cannot exist and be observed without selection. The parameter M quantifies a_M as an *epistemological limit*, set by the resolution of our measuring devices. In the limit $M \rightarrow 1$, where the resolution of measurement is *exactly one object*, the threshold a_M becomes an *ontological limit*, a_1 . This captures the maximum expected assembly index for the existence of any object, where $\langle n(a_1) \rangle = 1$. For most systems of interest, due to

exponential branching of the space, the epistemological and ontological limits will be quite close (see e.g., **Figure 2**).

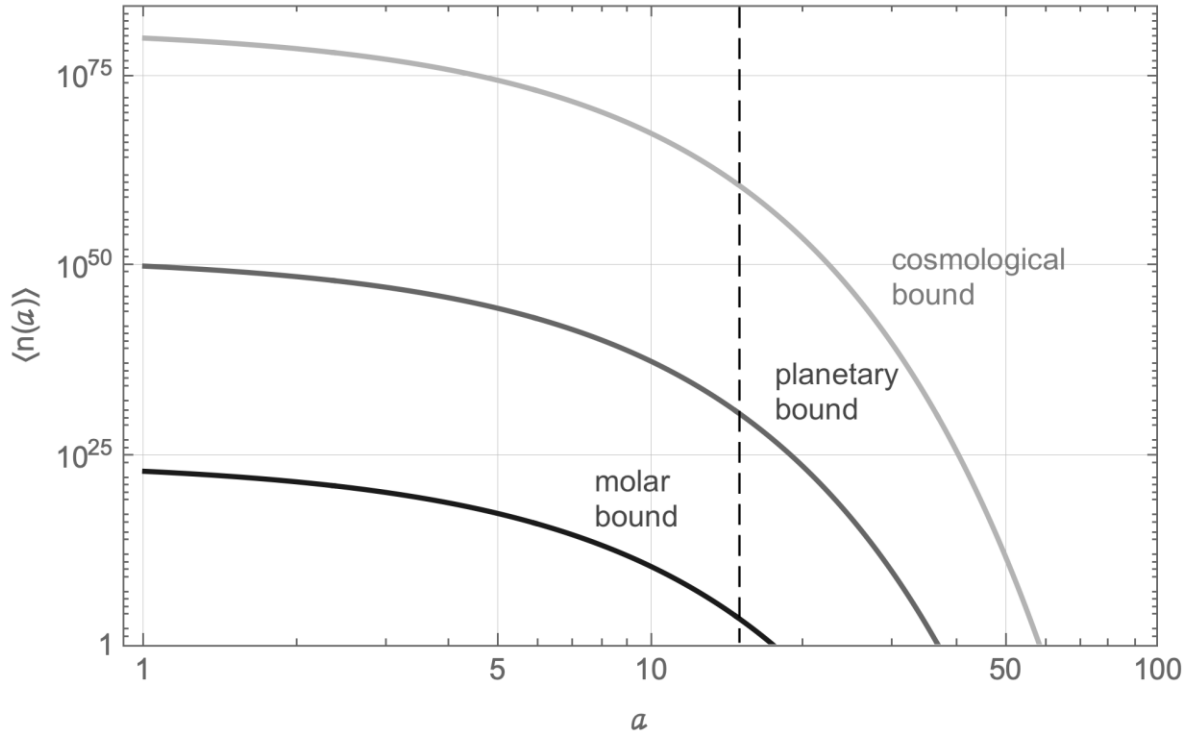


Figure 2. The expected copy number of objects at a given causal depth, quantified in assembly time, a , for varying volumes of total material. For the curves shown, $N_T = 10^{23}$ (1 mole of material), $N_T = 10^{50}$ (approximate number of atoms composing the Earth), $N_T = 10^{80}$ (approximate number of atoms in the observable universe). The value of the branching factor, b , was set using the experimentally determined threshold value of $a_M = 15$ determined in Marshall et al.²⁴ (dashed line), where no molecules with assembly indices $a_i > 15$ were detected in molar samples of abiotically-derived material, with a detection limit of approximately 10,000 molecules in the mass spectrometer used in the measurements. Using Eq 1. with $a_M = 15$, $N_T = 10^{23}$ (~ 1 mole), and $M = 10,000$ yields an approximate averaged global branching over small molecule organic chemical space of $b \sim 25$ from our simple model. With $b = 25$, we can extrapolate to different volumes of material, to determine the scaling of a threshold value of a_M where the ontological bound is achieved, that is where $\langle n(a_{M=1}) \rangle = 1$. For a molar sample of abiotic material $a_1(10^{23}) \sim 18$, the planetary bound is $a_1(10^{50}) \sim 37$ for an abiotic system with roughly as many molecules as there are atoms on Earth, and the cosmological bound is $a_1(10^{80}) \sim 58$ for an abiotic system with roughly as many molecules as there are atoms in the observable universe. Although these are very rough estimates, this demonstrates the existence of a cosmological bound and implies it is possible to extrapolate from laboratory based measurements to make predictions such that *any* molecule with $a_i > a_1(10^{80}) \sim 58$ is a signature of a deep causal history of evolution and selection; these cannot form spontaneously even leveraging the volume of the entire universe.

The branching factor satisfies $b \geq 1$, where the limiting case $b \rightarrow 1$ occurs only if each object can undergo only one causal join and can make only one new possible object. In chemical space, where the combinatorics of new bond formation scales *at least* exponentially with the molecular size, b is expected to scale exponentially with a_i , and the bound presented herein is a gross underestimate of the combinatorics. However, given that experimental data suggests only small a_i molecules exist abiotically¹⁸, a constant b provides a reasonable first approximation.

The ontological threshold, a_1 , defines a natural division between spontaneous and selected objects, with important implications (here i indexes distinguishable objects):

1. Objects with assembly index, a_i , below the threshold ($a_i < a_1$) can arise spontaneously and could exist in abundance anywhere conditions permit.
2. Objects with assembly index above the threshold ($a_i > a_1$) require specific causal histories and *cannot* arise without selection.
3. Observing high copy numbers of high assembly objects ($a_i > a_1, n_i > M$) is a signature of selection along a deep causal lineage.

The threshold is weakly system-size dependent, see **Figure 2** (e.g., it does not change by even one order of magnitude going from laboratory to cosmological scales). The dependence on the number of countable objects in a sample renders a_M an *extensive physical variable*, which is both substrate dependent (via branching, b) and volume dependent (via system-size, N_T). This allows setting bounds on a_M for laboratory samples, and using this to determine planetary and cosmological bounds, see **Figure 2**. The cosmological molecular bound considers an upper limit on the number of countable molecules in the observable universe using the estimated number of atoms ($N_T \sim 10^{80}$), which suggests that *any* molecule observed in abundance with $a_i \gtrsim 58$ must be a signature of a deep causal history of evolution and selection; these cannot form spontaneously even leveraging the countable volume of the entire universe. For reasons stated we expect this to be an overestimate, in particular because (1) the

assembly space grows much faster than accounted for here, (2) the number of molecules in the universe will be smaller than the number of atoms, with the number possible decreasing with molecular weight and (3) the mass is distributed over the entire universe and not within a reaction volume. Future work can include more realistic assumptions, and more experimental data, leading to tighter bounds and predictions from the theory. Our example here is intended to be simple enough to show a critical role for both assembly index and copy number, combined with an ontology of microphysical causation, as necessary to defining a universal threshold for detection of the constructive causal lineages more colloquially referred to as ‘life’ and/or ‘intelligence’.

Assembly Space

The above argument is well-defined within assembly space. Assembly space defines all possible objects constructable from basic units via recursive causal joining steps²⁴, and all the pathways connecting them. That is, assembly space encodes causal possibilities as a physical space that can be metrologically explored. In AT, the assembly space is a physical space that objects exist in, just as objects exist in spacetime in more familiar physics. Assembly spaces are substrate specific^{18,25–27}, which we shall discuss in more detail later, here we introduce a general definition, following²⁸.

Definition 1 - Assembly Space. An assembly space (Ω, U, J) consists of, Ω , its set of possible objects, $U \subset \Omega$, the set of elementary units for assembling objects, and possible causal joins $J: \Omega \times \Omega \times \Omega \rightarrow \{0,1\}$, where $J(x, y, z) = 1$ indicates the causal join can happen such that objects x and y can be assembled to form object z , e.g., $\{x, y\} \rightarrow z$. The assembly space Ω is the closure of U under all joining operations J , meaning Ω contains all possible objects that can be constructed from the set of basic units U through any sequence of possible causal joins. For combinatorial, compositional spaces, like chemical space, languages, memes, and morphologies, the full assembly

space is not computable and not physically realizable. What we can know about the structure of assembly space is determined by deconstructing (fragmenting) observed objects.

The assembly space has several important properties. It is combinatorially constructed, such that many parts can combine in many ways. It is recursive, such that objects are only possible to assemble with the products of preceding steps along causal chains. These features establish assembly space as a *causal possibility space* and one that unifies both dynamics and objects, which have traditionally been considered distinct in other physical ontologies. See for example, Walker and Davies²⁹ for a discussion of a need to unify states and dynamical laws to arrive at a physics descriptive of life. AT collapses the distinction between the two. The structure of the assembly space makes no distinction between sequences of causal joins and the objects they assemble; objects are causal chains.

Possible futures are causally open and undetermined, but the possible past is causally closed and trapped in existing objects. Consistent with this physics, what can be known about what is possible can only be determined from existing objects. Thus, the assembly space is derived from the deconstruction of objects: the units and joining operations are determined via recursive fragmentation of observed objects. We define fragmentation as the process of splitting an object into two parts, e.g., $z \rightarrow \{x, y\}$. By symmetry and invariance of physical laws³⁰, the inverse causal operations of joining the two objects must then also be possible, defining the joining operations and the assembly space, see e.g. Marshall for molecular assembly space^{18,31}. We note the physical circumstances in the environment mediating a fragmenting process or joining process need not be strictly equivalent, for example it may require human-level intelligence to make a highly symmetric DNA nanostructure, but the molecule could be broken by the ordinary process of phosphate ester hydrolysis. Thus, the symmetry of causation we invoke here does not imply the reverse (fragmentation) and forward

(joining) environmental constraints are symmetric (see e.g., Marletto and Vedral for an example of similar asymmetry in fundamental physics³²). Instead, here symmetry and invariance imply the causation *in* the material (fragmenting/joining) *is* symmetric. One arrives at units when an object produced by a particular mechanism of fragmentation (e.g., such as breaking bonds) can be fragmented no further by that same mechanism, defining the boundary of a ‘substrate’ in AT. The causal symmetry within objects has potentially deep implications for this physics given the connection between invariance and symmetry³³, a subject we leave to future work.

To uncover the structure of assembly space two requirements are necessary. First, one must identify the bounded, distinguishable structures of a substrate, defining its objects. Second, a measurement scheme must be identified that can interrogate how objects can be fragmented recursively to units. From units, paths are re-assembled via causal joins to find the minimum number of steps to arrive at the observed objects.

Consistent with the definition of objects in AT (see Sharma et al.¹⁷), what we call ‘objects’ in the assembly space are strictly those observed to exist in high enough copy number to be measurable³⁴. Thus, it is the termination of lineages of causal steps in the assembly space, where there is a high copy number at the terminus, which is definitive of the objects we observe, see **Figure 3**. All other structure in the assembly space is what we call ‘*virtual objects*’: their identity is defined based on the existence of objects, e.g., via the process of fragmenting those objects and re-assembling them. Virtual objects have no autonomous existence, because there does not necessarily exist a causal mechanism that can produce identical, countable copies of these structures in high numbers. Using mass spectrometry as an example, for complex molecules millions of fragments might be produced for an individual molecule, and it is not necessarily the case that any one of these can be generated reliably. Nonetheless we can infer the existence of the assembly space via these fragments, as virtual manifestations of it.

The definition of an assembly space is predicated on objects being deconstructable in a finite sequence of causal steps. In the prevailing conception²¹ of reductionist physics, breaking apart physical systems is understood to reveal something of the physics that binds objects into higher-order structure. For example, removing electrons from an atom reveals properties of Coulomb interactions between the negative electrons and positively charged nucleus. This has led to a standard explanatory interpretation in the form of physical laws that exist outside of objects and somehow dictate their behaviour³⁵, leaving open the question of what ‘breathes fire’ into these equations to yield a universe for them to describe as articulated by Hawking³⁶. In AT, we view the reductionist insight differently, as it reveals a more general property of all objects our universe constructs: the causal constraints from which an object can be assembled are *intrinsic* to that object. There are no external ‘laws’. This sets the foundation for defining the assembly index as an intrinsic measure of causation, leading to assembly index as a proposal for complexity as an ontological property (see e.g., Lloyd³⁷ for other categories organizing prior approaches to complexity across different fields).

Causation

An axiom of AT is that objects *require* a causal sequence of steps to exist. Indeed, objects *are* a causal sequence of steps. Thus, there must be a minimum number of steps as a necessary property for the existence of any object. As we have noted, this physical property of each distinguishable object type, i , is quantified in its assembly index, a_i . Assembly index is an *intensive* property, subject to measurement, independent of formation history, system size or measurement method (see section on measurement). We now define it more formally²⁸.

Definition 2 - Assembly Path and Assembly Index. An *assembly path* is a finite sequence of causal joins,

$$\{(x_1, y_1, z_1), \dots, (x_n, y_n, z_n)\}$$

that satisfy: $\forall i \in \{1, 2, \dots, n\}, x_i, y_i \in U \cup \{z_1, z_2, \dots, z_{i-1}\}$ and $J(x_i, y_i, z_i) = 1$. That is, for any object $z \in \Omega$, an assembly pathway for z is defined as a finite directed acyclic graph whose leaves are labelled by elements of U , whose internal nodes represent causal join operations J , and all join operations in the pathway ultimately produce a single final object z . For any object, $z \in \Omega$, the *assembly index* of that object, denoted $a_i(z)$, is the number of causal joins along a shortest assembly path that has z as its final product. If $\{(x_1, y_1, z_1), \dots, (x_n, y_n, z_n)\}$ is a shortest assembly path for z , then $a_i(z) = n$. For a canonical choice of primitives, composition rules, and object equivalence, the assembly index is a well-defined property of the object.

While it is simple to write out an assembly pathway as a labelled sequence, doing this in a causally relevant way to reveal the structure of the assembly space is non-trivial. Joining operations in an assembly space are substrate-specific and must encode causation as it operates in that substrate. For example, in molecular assembly space, hydrogen atoms are typically not treated as explicit assembly primitives, because including them adds substantial combinatorial complexity without increasing discriminatory power in practical measurement or in the calculation of molecular assembly index²⁸, but for atmospheric assembly space they are critical²⁷. The assembly space of solid state materials has yet a different structure²⁵.

The formalization of assembly index captures:

- (1) **Causation.** Assembly index counts the minimum number of causes (joining operations) to produce the object.
- (2) **Contingency.** Only structures constructed along an assembly path are available for recursive use to construct subsequent objects.
- (3) **Invariance.** Assembly index does not depend on the identity causal joins or their precise ordering, only the shortest countable number to assemble an object, which is a path-independent feature of the object.

The assembly space introduces a material and intrinsic concept of causation, because it encodes the direct influence of one component on another's possible existence, see **Figure 3**.

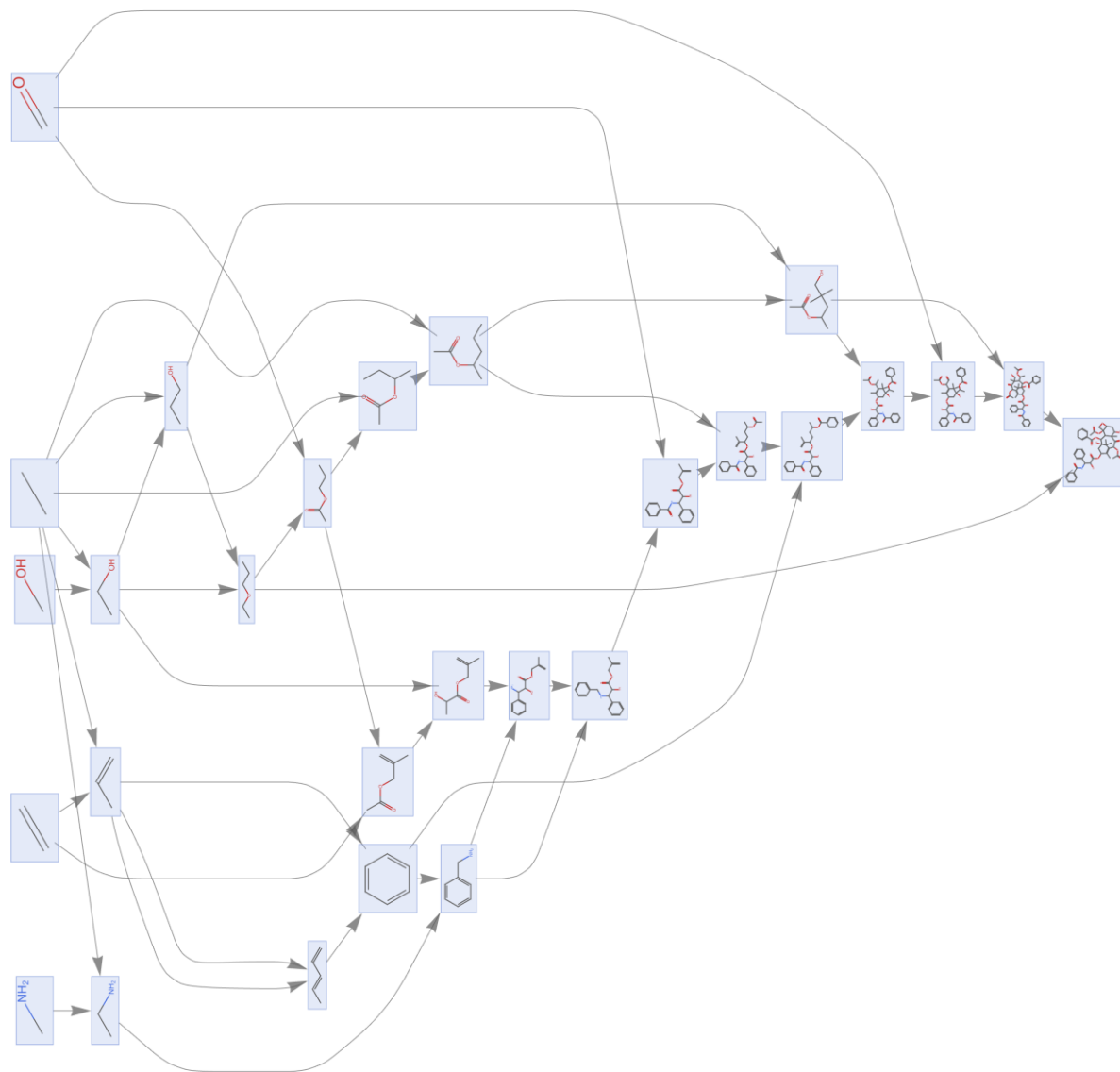


Figure 3. Assembly pathways reveal the materiality of causation, where each object within an assembly space exists as a sequence of causal joins on a minimum path where we observe a high copy number at the terminus. Shown is a minimum assembly path for Taxol, which has 23 steps.

This dissolves issues inherent to counterfactual definitions of cause^{38,39}, such as the need to iterate over interventions that cannot be fully specified or computed. The restriction of steps along an assembly path to joining operations implicates these as

fundamental units of causation, and yields a precisely defined, and material concept of 'cause'. Causes are structures that appear on a minimal path to construct an observed object. It is worth noting that these structures are causal joins of two fragments, that these are not *a priori* labelled, and their precise identity as virtual structures need not be known.

A causal join must exist before its product can be used, imposing a measurable partial ordering on the existence of objects with testable consequences. This yields an ontology where objects include causal extent as a material attribute. Complex objects of the kind we interact with in biology and technology are effectively hyper-objects as their assembly space, or lineage, is large in its causal depth.

It is not trivial to determine what set of circumstances allows one object to exist over another⁴⁰. The mediators of contingent causal chains are sometimes referred to as 'constructors'^{20,21}, but this concept is often so abstract as to be poorly defined. Many constructors of interest are too largely distributed in space and time to be useful for theoretical and empirical interrogation. For example, the (symbolic) laws of gravitation are a component of the constructor necessary for artificial satellites to orbit Earth – but this constructor also includes engineers, factories, rocket propellant and a myriad of uniterable, but finite, other objects that exist in our biosphere³. Constructors can be massively distributed in space and time, often hidden from our direct perception (for example, often we do not recognize math, symbols or languages as physical objects⁴¹).

The universe itself is one such concept – we will never observe all of it at once (being contained within it), so we will only ever be able to discuss it in the abstract. In this sense the very idea of "universe" is itself an emergent property of all the causation we can observe constructing things into being. Measuring causation that is large in its spatial and temporal extent presents a challenge, and indeed, is at the heart of the

challenge in measuring the emergence of new lineages from non-living substrates (the origin of life). In AT, we recognize it is not possible to precisely define nor measure the presence of large constructors directly. It is possible to measure the shadow of a constructor in the object(s) it generates (see also discussion on connection between AT's concept of cause and Derrida's deconstructivist concept of trace, as explored by Mastrogiovanni⁴²).

Constructors are not physical in a material sense, but assembly spaces are. Attempts to formalize life have frequently focused on immaterial concepts of information⁴³. AT is the first to define the physics as material and does so in recognizing causal possibilities as a physical space, the assembly space. This underlies AT's unique definition of material causation. It introduces an ontology where hierarchy is defined in terms of the possibility to exist, radically departing from notions of hierarchy defined in spatial or energetic scales found in other theories (see Ardoline⁴⁴).

Contingency

Observing *any* distinguishable object in discrete copies provides direct evidence that the universe contains a causal mechanism to produce (and reproduce) that same object. Copy number is evidence of stored memory. This is distinct from frequentist approaches to probability, where frequency is used as evidence something is likely⁴⁵ (see Appendix A). Copy number allows formalizing contingency along causal chains within the assembly space by capturing dependency on prior selective steps.

Definition 3 - Copy number. Copy number, n_i , is the countable number of each distinguishable object type, i , (defined up to limits of measurement).

In AT, copy number is *not* related to the probability for the object to occur, which is, in general, not definable (see Appendix A). Instead, copy number is an indication of

contingency in the causal chain that allows the object to exist at all. This is sufficiently important that it is a principle of AT:

Copy Number (CN) Principle. The existence of countable copies of a distinguishable object type is direct evidence of contingency along the causal chain mediating the object's construction.

The copy number (CN) principle is inclusive of mechanisms that are spontaneous. Processes that can occur everywhere (spontaneously) are often captured by what we call "physical laws" that aim to explain such universal regularities. But the CN principle is broader than universal laws in physics, because it also applies to all non-universal causal regularities, inclusive of high assembly index objects and not just the low assembly index ones. Some mechanisms of causation (indeed most if we consider the full space of possibilities) are contingent and *not* spontaneous, and they are therefore not found everywhere in the universe. Ribosomes provide evidence of one such local causal regularity or 'law-like' process that may only exist on Earth: the constructive context known as a biological cell. Ribosomes have persisted in high copy numbers on this planet for billions of years⁴⁶ because there is a localized physical system (the cell) which allows their reliable, reproducible construction. The copy number of ribosomes on Earth is not evidence of the universal probability of their formation, but instead is evidence of a contingent causal chain persisting on Earth (see Appendix A).

Measurement

Although it is now common knowledge as statement of scientific fact that water boils at 100°C, this statement is not true of the world. Water boils at slightly different temperatures if it is in a glass container versus a metal one, if it is aerated or not, depending on what altitude you are at, etc. The standardized temperature scale came

about because of the invention of a theoretical abstraction, the concept of absolute zero, originally defined as a fundamental limit to the degree of coldness possible⁴⁷. By reference to this theoretical limit, all other (hotter) objects can have their relative temperature defined precisely. This scale works even if absolute zero is not a physically attainable temperature.

What if there could be a similar standardization, not for a temperature scale, but for the measurement of causation? The assembly index is structured to provide such a standardization, such that each object a_i , and the substrate-specific and measurement specific a_M , can be determined experimentally. We will describe the metrology of AT as developed for molecules as a special first case of application of the metrology of the theory.

For molecules, measurements have been done using techniques where the number of parts within a molecule can be determined using standard laboratory methods, like infrared (IR) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, and mass spectrometry (MS)⁴⁸. These techniques rely on different types of experimental data, yet have each been found to give evidence for the direct measurement of molecular assembly index.

Assembly theory was first developed by one of us (Cronin) via thought experiments about measuring causation in molecules using mass spectrometry. In a chemistry lab, mass spectrometry is a common technique for identifying molecules and measuring their properties⁴⁹. This works by shattering molecules into fragments, giving characteristic patterns for specific molecules based on the charge-to-mass ratio of the fragments produced. Thought experiments leading to the development of the assembly index were inspired by this fragmentation process, and how one could reassemble a molecule in successive steps by sticking the fragments back together, ensuring any redundancies are removed to guarantee the smallest number of joins^{18,24}.

If some fragments are identical and can be reused, fewer total steps are necessary to reassemble the original molecule. This is indicative of the inherent, physical hierarchy in how to count constructive complexity that came to underlie the assembly index as a measure of intrinsic causation.

This process mirrors the formalism of assembly space and the assembly index, so it is tempting to say that assembly index is just a correlate of the mass spec fragmentation. However, this is demonstrably not the case. For a given molecule the complete quantum state (or equivalently its ground-state) contains *all* information about bonding, connectivity, symmetry, and repetition. This can be ‘read-out’ by the spectroscopic techniques of mass spectrometry, NMR, and Infrared. Any of these techniques can be implemented to determine assembly index because the assembly index is a functional of the quantum state of the molecule, which measures the minimum generative description length of the molecular graph under physically allowed composition rules. Before AT, this functional was simply not identified, formalised, or measured. What makes assembly index new is not that it adds information to quantum mechanics, but that it selects a particular invariant that had no prior analogue in physics. The assembly index is global, not local (unlike energy, charge density, or force constants), it is non-extensive (copying a module does not increase it linearly), and it is algorithmic, not additive. The assembly index is observer-independent once the construction rules are fixed. Finally, it is experimentally accessible through lossy projections (IR, MS, NMR) without full structure reconstruction⁴⁸. This is why IR, MS, and NMR can all be used to measure the assembly index, using radically different physical mechanisms and instrumentation. These techniques are not measuring the same thing directly; they are however all projecting the quantum state through different symmetry, and redundancy preserving, channels. The same scalar emerges robustly across these orthogonal probes providing the strongest evidence to date that assembly index captures something intrinsic rather than an artefact or some kind of heuristic. This provides a

newly identified intrinsic physical invariant of molecular structures, consistent with quantum mechanics but not recognised, nor experimentally operationalised until the advent of AT.

Thus, via the assembly index, the concept of ‘causation’ in AT becomes a feature like charge, spin or other quantum numbers, or the speed of light c . It does not depend on the object’s environment, reference frame, or measuring device. Although this is a strong claim, it has been rigorously tested. If the assembly index were not intrinsic, it would depend strongly on representation, spectroscopy choice, or observer-dependent assumptions. The empirical fact that it survives IR, MS, and NMR, all with different physics, different noise, and different symmetries suggests invariance⁴⁸.

This invariance is critical to the metrological standardization of constructed complexity of molecules, which is a necessary step towards experimental confirmation of an abiotic upper limit setting a threshold for life detection. To confirm a threshold, measurements must be taken for objects derived from living and non-living samples, with an understanding that the threshold value is system size dependent $a_M(N_T)$. For a laboratory mass spectrometer, the copy number of identical molecules sets a detection limit of $M \cong 10,000$ because this is the lower limit of detection, see **Figure 4**. We show this detection limit set against the abiotic assembly copy number distribution in **Figure 4**, showing how determination of an abiotic threshold in assembly space depends on both system size and instrument resolution. The existence of a threshold has been demonstrated experimentally in Marshall et al.¹⁸

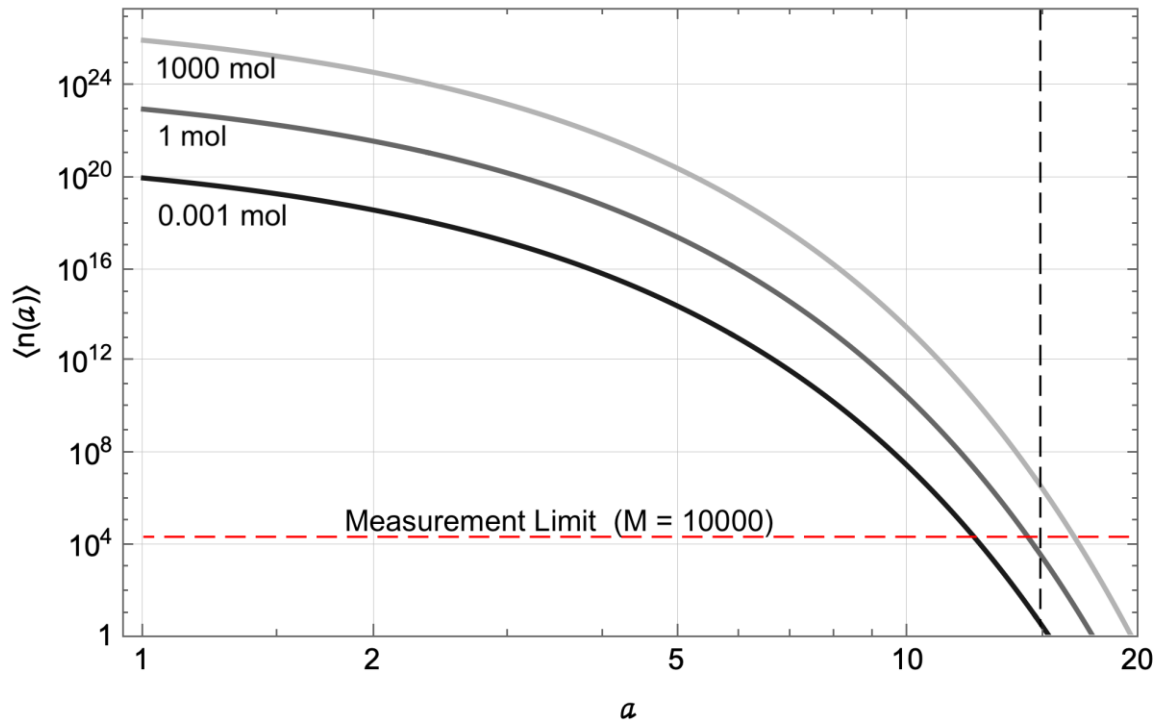


Figure 4: The epistemological limit set by a measurement device determines the maximum assembly index object expected to be observed in the absence of selection. Shown is the measurement resolution for a mass spectrometer, where a minimum of $M = 10,000$ identical molecular objects must be present (horizontal red dashed line), relative to the abiotic copy number distribution for laboratory scale samples ranging from $1/1000^{\text{th}}$ of a mole to $1,000$ mole. As in Fig. 2, we set $b = 25$ to be consistent with experimental measurements in Marshall et al.²⁴, which set the limits of detection of abiotic molecular complexity at $a_M = 15$ (vertical, black dashed line) in molar samples. In Fig 2., there is no measurement cut-off, but here we show how the tail of the distribution will be below the measurement cut-off for most experiments, rendering the two distinct phases (spontaneous or abiotic, versus selected or life) more obviously distinguishable by an abrupt discontinuity (see e.g. Marshall et al.²⁴ where the cutoff at $a_i = 15$ is abrupt). For the simple model presented, a value of $a_M \sim 18$ is expected for experiments on abiotic systems with 10^3 mol of material, a prediction which should be refined with more detailed analyses of the structure of molecular assembly space and its branching.

Selection

We are now in position to define the *assembly* of a system, which quantifies the total amount of selection among causal possibilities required to generate and maintain all objects in the system. It combines both the material causation of objects (assembly index) and the evidence of persistent contingent causal mechanisms (copy number),

allowing a formalization of phases of matter associated with abiotic and living (or intelligent) objects.

We call the configuration of causal possibilities intrinsic to a collection of objects an *assemblage*, where the total causation is quantified by its Assembly as:

(3)

$$A = \frac{1}{N_T} \sum_{i:n_i>1} n_i e^{a_i}$$

where n_i is the copy number and a_i is the assembly index of the i th distinguishable object type. This equation captures how producing few copies of a complex object requires more selection and contingency along causal lineages, than producing many copies of a simpler object.

A configuration in standard physics is formalized to capture the current position and momentum of a system. This should be considered only as the current time slice of that configuration's assemblage: the assemblage includes the accumulated causal possibilities, recursively assembled to generate the configuration. The assemblage is a causally deep representation of matter.

We take as an axiom that any object with assembly index $a_i > 1$ cannot be realised without the existence of objects of lower assembly index along at least one minimal assembly pathway; that is, every object observed with assembly index $a_i > 1$ exists both in the physical objects we count and interact with, and as a virtual space of finite support that encodes the underlying causation necessary to its existence. Each object observed implies the realizability of a hierarchy of objects causally prior to its existence. The quantity A makes this implication explicit, defined by introducing a *virtual copy number*, v_i , that compounds copy number through recursive composition of causal chains, e.g., the assembly paths. To derive this for an observed object, we

start at the base of its assembly space with an object of zero assembly index carrying a unit weight and add causation equivalent to compounding following all branches into the one realized causal join at each step. Over an assembly path terminating at an object with assembly index a_i , each step collapses b possibilities, and this yields a virtual copy number:

$$v_i \propto \left(1 + \frac{1}{b}\right)^{b a_i}$$

Here, b is similar conceptually to the branching parameter we described earlier but can now be understood as the number of discrete causal steps that *could* be taken, out of all possibilities, for each unit increase in assembly index, recursively compounding copy number along contingent chains. This allows quantification of causation in the number of possible branches that must have collapsed into each actualized causal join over all steps culminating in an object. Here assembly index plays an analogous role to time, with b determining how much causation compounds per unit assembly time.

For an observed object of type i , with n_i copies, the causation quantified in the virtual copy number is weighted by its contingency in the copy number of observed objects at its terminus, yielding the virtual copy number

$$v_i = n_i \left(1 + \frac{1}{b}\right)^{b a_i}$$

Earlier we assumed a branching term was finite for each physical object. Here, in the virtual parts of assembly space we must contend with how the environment is unresolved, not deterministic, and not discretized until selection operates to fixate specific causal mechanisms (objects) into existence. Thus, against this unresolved virtual background of causal possibilities $b \rightarrow \infty$ and the above becomes

(4)

$$v_i = n_i e^{a_i}$$

such that the virtual copy number captures how the number of objects observed encodes a lineage of selected causation in its virtual objects. Summing over an entire assemblage yields the total virtual copy number of the population:

$$v_{\text{tot}} = \sum_i v_i.$$

And finally, the assembly, A , of a population is the total virtual copy number per observed object,

$$A = \frac{v_{\text{tot}}}{N_T} = \frac{1}{N_T} \sum_{i:n_i>1} n_i e^{a_i}$$

Thus, A represents a density in causal depth per observed object. The restriction to object types with $n_i > 1$ implements the copy-number principle: repeated occurrence is necessary to evidence a reproducible, selected causal generative process rather than a fluctuating contingency.

Assembly is *extensive*, and scales with system size (total number of objects). It is also measurable because both n_i and a_i can be experimentally determined. It captures cumulative selection because it accounts for both the causal depth of objects in a combinatorially explosive space (assembly index) and the persistence of the mechanisms to produce these objects (copy number).

This formulation allows us to quantify when systems undergo transitions from abiotic chemistry to life-like behavior. As a system accumulates more complex objects in higher copy numbers, its A increases. Systems above a critical threshold in A mark a phase transition in assembly space, where some of the $a_i > a_M$, and contingent lineages of virtual objects are necessary to support existence. This is when objects we observe can be causally deep in the assembly space. Such objects are expected to exhibit properties commonly associated with living and intelligent systems, including persistent complex structure, reliable reproduction, and potential for agential and

open-ended behaviour, features which we regard as arising because of their deep virtualization in the space of causal possibilities.

Open-Ended Evolution, Novelty and the Mechanism of Selection

Assembly operates on discrete objects whose identities and assembly indices are defined retrospectively, while interactions occur in a continuous or unresolved space that is not discretised in advance before selection fixes causal mechanism. Novelty emerges when such interactions produce outcomes that do not map onto existing object types. Most such outcomes are transient and leave no causal trace. Persistence enables repeated interaction with the same unresolved region of possibility space, justifying its discretisation to a new physical object type. Once discretised, the object becomes part of extant causal memory and constrains future interactions. Assembly index records the depth of this accumulated causal memory. This provides a mechanism for open-ended evolution, where open-endedness emerges from an asymmetry between discrete causal memory and an under-resolved environment. Open-ended evolution therefore arises not from randomness, but from delayed discretisation of continuous interactions filtered by persistence and reuse.

Assembly theory treats a population of objects as a discrete causal memory embedded in an undetermined space. Each object i is characterised retrospectively by an assembly index $a_i \in \mathbb{N}$, the minimum number of joining operations required to construct it, and a time-dependent copy number $n_i(t)$, with $N_T(t) = \sum_i n_i(t)$. Assembly index encodes causal depth but does not predict which objects will appear.

Novelty arises when interactions between the current assemblage and its under-resolved environment generate outcomes not previously present; these outcomes are only discretised into new object types if they persist and recur, because only then can their identity be indexed and measured.

Depth and persistence are connected via the virtual copy number. One copy of an object at assembly index a implies an exponentially growing causal structure supporting the existence of the object, so we associate to each object type, i , a virtual copy number $v_i(t) = e^{a_i} n_i(t)$. The assembly becomes time-dependent in the normalised virtual burden carried by reproducible objects,

(4)

$$A(t) = \sum_{i: n_i(t) > 1} e^{a_i} \frac{n_i(t)}{N_T(t)} = \frac{1}{N_T(t)} \sum_{i: n_i(t) > 1} v_i(t),$$

which quantifies how much causation is instantiated per observed object.

A discovered object may exist transiently with $n_i(t) > 0$ yet remain causally sterile; it becomes causally effective only if it persists long enough to be used to propagate formation of structure. This means the objects persistence time τ_i must be long enough for the copy number to increase, e.g. such that $n_i(t) \geq 2$. Causation at assembly index a_i requires this persistence time to exceed the characteristic waiting time, t , for reuse in the combinatorially expanding assembly space such that $\tau_i \gtrsim t_{a \rightarrow a+1}$. When this condition holds, the virtual copy number causal burden per object e^{a_i} implies the causation is trapped once and reproduced through reuse; when the condition fails, the burden must be repaid upon each rediscovery, and the object cannot contribute to propagating causation to contribute to sustainable growth in assembly index.

This leads to an expansion and contraction of the assembly space. When new objects are constructed, they expand the assembly space itself, enabling construction of even more complex objects. This can yield a “ratchet” effect where each new object opens new possibilities, and the extinction of objects closes off possibilities. In expansion phases, the threshold recedes allowing spontaneous combination to make more complex things than in the absence of a deep lineage. In contraction phases, the threshold drops back, returning to the abiotic value in the absence of any deep

lineages. Thus, the assembly space is not static but dynamic, becoming larger as new causal mechanisms emerge and smaller as objects die out. The new causal mechanisms cannot be predicted *a priori*, and mechanisms are only predictable so long as they persist.

AT provides a testable mechanism for open-endedness following from delayed discretisation at the interface between discrete memory and continuous possibility. Interactions continually sample an outcome space that cannot be enumerated in advance; most outcomes vanish without leaving a trace in $A(t)$. Those that persist are stabilised, labelled as new object types (with a_i defined only after the fact), and incorporated into the assemblage, increasing the mass of reproducible high- a objects and allowing the high-end tail of the assembly-index distribution to ratchet upward over time only under certain selective circumstances (e.g. as governed by persistence time of objects).

Selection acts forward on persistence and copy number, while causation accumulates backward through assembly index, and their coupling is made explicit by the joint dependence of $A(t)$ on a_i and $n_i(t)$. In other words, any genuine, novel, open-ended process does not have objects that can be defined before the universe constructs them, captured in the ontology of AT in how the assembly space can only be determined relative to observed objects. There is no definable, global assembly space that exists outside the objects we observe, enabling a physics describing a universe that is self-constructing.

Deterministic dynamics and predictability are emergent properties of the assembly space: more objects become predictable as objects grow deeper in the assembly space because the space itself will encode more causal mechanisms. Many physical processes can be simulated algorithmically after the fact, but open-ended evolutionary

processes cannot be fully characterised as closed computations over fixed symbols and rules. The reason is structural because the identities of relevant objects and operations are not fixed in advance but emerge retrospectively through persistence and reuse. The effective state space therefore expands over time in a way that cannot be enumerated *a priori*. Any finite history can be simulated retrospectively, but no single closed algorithm can predict in advance which new objects will arise, persist, or become causally significant. This reflects delayed discretisation and state-space expansion.

What AT explains, then, is how evolution and selection allow ‘compactifying’ larger volumes of causal possibility within smaller volumes of physical space, increasing the virtualization of objects as they become deeper in assembly space, that is, as ‘life’ or ‘intelligence’ carve deeper trajectories into what is possible.

Entropy and Assembly

To understand assembly as a physical quantity, we can relate it to more familiar concepts like entropy. From our discussion on measurement, it should already be apparent that assembly index is unlike entropy, as it is not an ensemble quantity. Assembly index is more like a topological or algorithmic invariant. Once the construction graphs are fixed, it is a property of the individual object (and therefore for molecules of the underlying quantum state that determines that structure). Assembly by contrast does play an analogous role to entropy, but for structured objects under construction, not for ensembles under thermal mixing.

Consider a toy example of two simple molecules with identical molecular formulae, $C_{11}H_{24}$, but different structures (they are structural isomers); 4-propanyloctane and 2,3-dimethylnonane. Assembly index can characterise the amount of causal symmetry in a molecule (how many steps are repeated), see **Figure 5**. Molecules with different

symmetries are also energetically distinguishable. The molecules 2,3-dimethylnonane and 4-propanyloctane have the same molecular formula, but differ in both their assembly index, which are $a = 5$ and $a = 4$ respectively, and in their heat of formation, which are -255.7 and -179.4 kJ mol⁻¹ respectively. The less symmetrical molecule has the higher assembly index and the higher heat of formation.

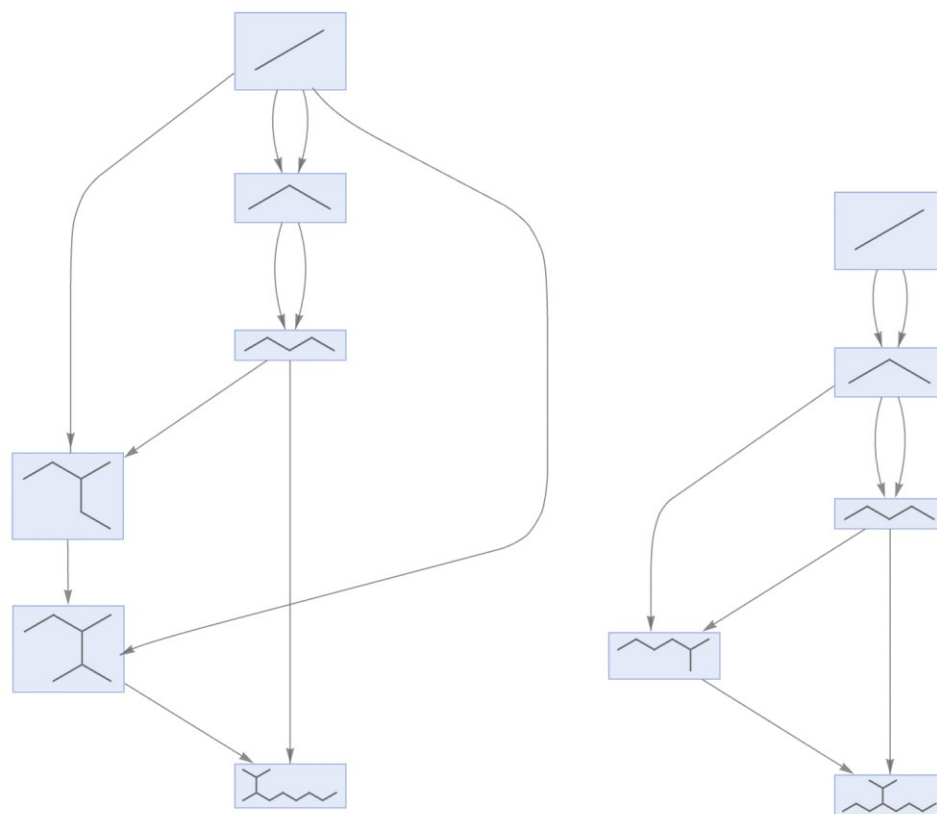


Figure 5. A minimum assembly path for 2,3-dimethylnonane (left), 4-propanyloctane (right). Both molecules have the same molecular formula, C₁₁H₂₄, and the same Shannon entropy for their smile representations; CC(C(C)C)CCCCC and CCCC(C(C)C)CCCC of 3.8 respectively. They differ in their physical properties including assembly index, with 2,3-dimethylnonane being $a = 5$ and 4-propanyloctane being $a = 4$ respectively, and heat of formation with 2,3-dimethylnonane being -255.7 and 4-propanyloctane being -179.4 kJ mol⁻¹, respectively.

Next consider the following thought experiment in which we assume the production of the molecule Taxol increases fitness, and hence the production of Taxol increases with growth and persistence of the Yew tree. A Taxol Demon represents the construction machinery that assembles the Taxol molecules using the gases as

reagents. The contribution to assembly, A , by Taxol will increase in a sigmoidal fashion, see **Figure 6**, representing the constructed order in the molecules, mirroring the decrease in entropy.

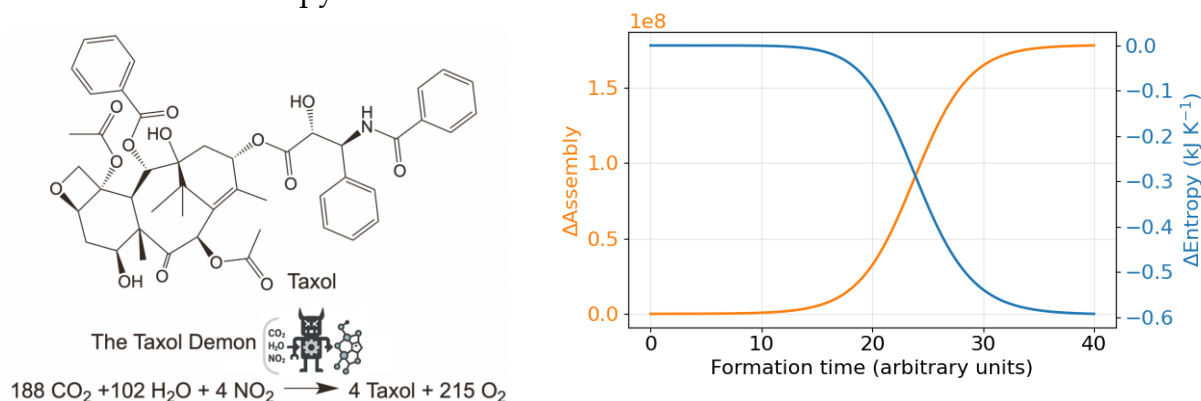


Figure 6. Left: A depiction of the process to construct Taxol from what would be its combustion products in oxygen, and the hypothetical Taxol Demon. Right: The increase in assembly (A) in Taxol. The entropy change of the system is depicted. With a change of assembly from 1.6×10^8 , the entropy of formation is $-3.8 \text{ kJ K}^{-1} \text{ mol}^{-1}$.

Recent advances in statistical physics have emphasized the importance of path-dependency in non-equilibrium systems^{50,51}. Assembly also formalizes a concept of path-dependency, which does not abstractly assume all possible paths are physically real, nor does it assume we need to experimentally select a path directly for it to be real (e.g. we do not assume context dependency to measurement of paths). The space of all paths cannot be exhaustively sampled (nor computed) in any real complex physical system of interest, suggesting it does not make physical sense to assign probabilities over these spaces: they are too large for even the entire universe to ever sample⁵². AT replaces the unphysical assumption of state spaces that cannot be sampled with a precise, finite definition of microphysical causation and contingency, which could provide an alternative foundation for path-dependency in non-equilibrium systems based on causal principles.

Causal Phase Transitions and Formalizing “Life”

We are now in position to discuss the nature of causal phase transitions within AT, and how these allow formalization of “life” characterized by persistent copies of objects in abiotically inaccessible regions of the assembly space. Causal phase transitions underlie persistence of objects beyond the threshold in its assembly space. As we have indicated, the assembly index for each object is intensive to that object, as it does not depend on the amount of sample. But A , and a_M are extensive, where both depend on the number of distinguishable objects N_T . The abiotic threshold a_M defines a critical surface in the space of possibilities, where any observed object with a larger assembly index than this, which persists in multiple copies, can only be produced via a selective mechanism. Because a_M is extensive, the assembly index of objects indicative of ‘life’ in the assembly space, will be system size dependent.

For each substrate-dependent assembly space, it should be possible to derive the conditions at a phase boundary, a_M , marking the upper limit of the complexity of abiotic systems, which will be system-size and substrate dependent. In general, our simple model presented earlier will underestimate the size of the possibilities because it assumes a fixed branching, when we should expect the number of possibilities to increase more quickly than a simple exponential with increasing assembly index. Nonetheless, we here use the simple model to also motivate some expectations about the phase behavior of A . Substituting equations (1) and (2) into equation (3) yields an effective description of A in the absence of selection:

(5)

$$A_{abiotic} = \left(b + \frac{1}{N_T} - 1 \right) \frac{e/b}{e/b - 1} \left[\left(\frac{M}{(1 - 1/b) N_T + 1/b} \right)^2 e/b - 1 \right]$$

Here the summation in Eq 3 is up to a_M , because for $a > a_M$, the terms are unobservable or zero. This is shown in **Figure 7**.

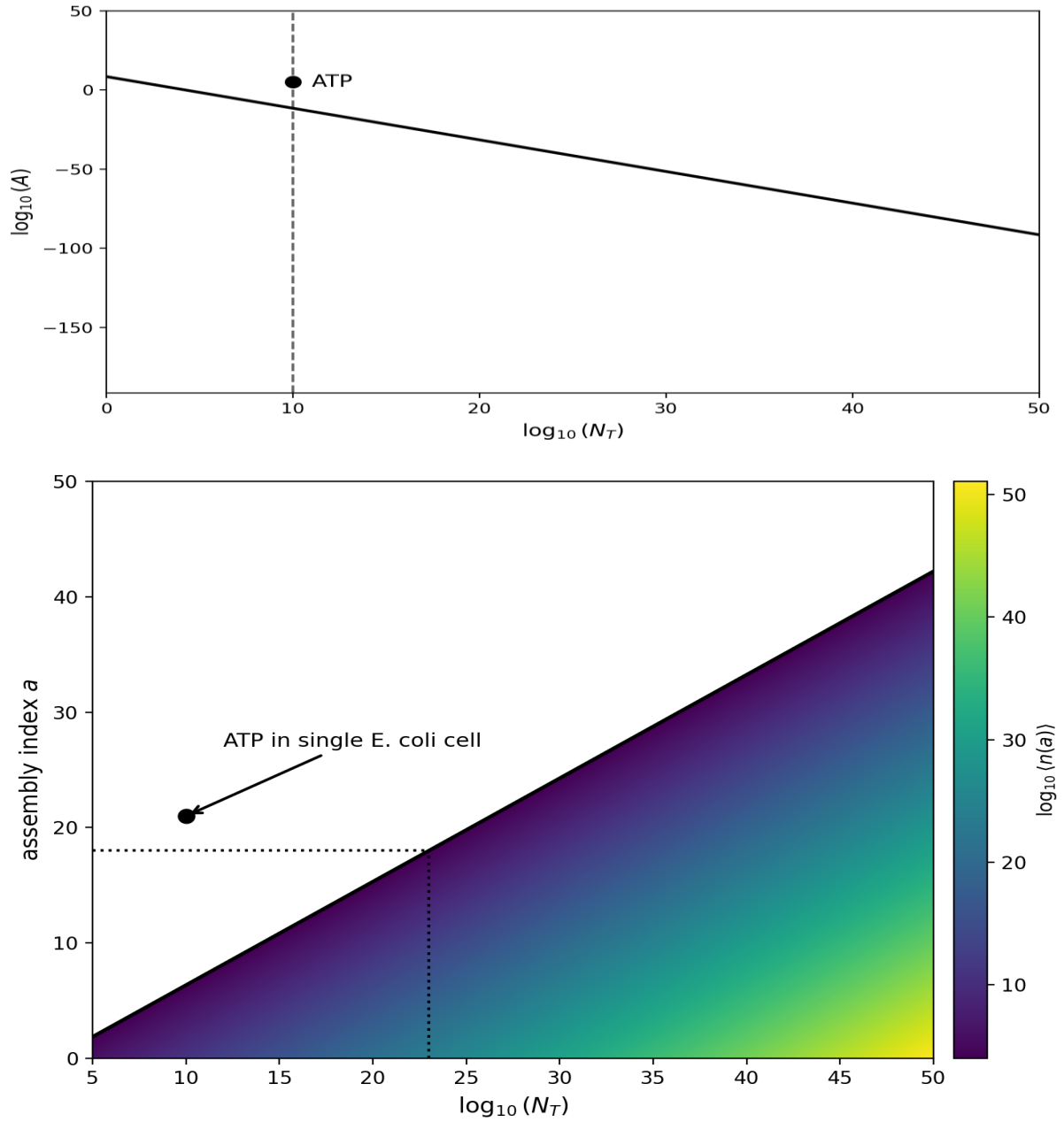


Figure 7: Top: The abiotic assembly A , consistent with a uniform copy number distribution over objects and a threshold a_M , decreases with the number of objects N_T . Shown is the distribution as a function of N_T and the assembly for ATP at concentrations found within a typical bacterial cell. Bottom: Abiotic copy number $n(a)$ as a function of a (y-axis) and N_T (x-axis) for fixed branching ($b = 25$, as above), with the line for a_M showing the division between objects expected to exist and those which are too assembled to exist in the absence of selection. The biological energy carrying molecule ATP, with $a_{ATP} = 21$ is plotted using its molar concentration within a typical bacterial cell, showing how its assembly index and number density in cells place it within a causal structure regime beyond the threshold and indicative of life.

In prebiotic chemistry experiments, molecules with $a > 15$ are sometimes observed⁵³. One might therefore consider that our argument must be flawed, and the empirical results already invalidated. However, it must be noted that *all* prebiotic chemistry experiments include some degree of selection, which comes in many forms ranging from using purified reagents, to controlling process conditions, to tightly controlling yield that are rarely reported, as well as introducing reagents with a high assembly index⁵⁴. It is an open question how to best parametrize and quantify these selective constraints⁵⁵. To be clear on the distinction, we use ‘*abiotic*’ in strictest definition of the chemistry that preceded life, which had no human influence or design^{56,57}. This leaves the term ‘*prebiotic*’ to be used to denote specific selective circumstances directed towards producing the molecules found in biology on Earth, as found in most current experimental efforts in prebiotic chemistry. That is, ‘prebiotic’ describes those cases where post-selection on extant biology is used to constrain experimental design on its origin (e.g. justifying the prefix “pre” denoting ‘before’ as in ‘predict’, whereas the prefix ‘a’ denotes ‘not/without’ as in ‘asymmetrical’). Prebiotic chemistry experiments represent significant selective constraints, placing nearly all experiments in the origin of life chemistry in the phase of causal structure associated to life, which is manifest in precise control by intelligent agents in the design and execution of prebiotic chemical experiments. Our hope is AT will open new paths towards proper bookkeeping of these selective constraints and the design of experiments that allow more minimal (and quantifiable) selective constraints such that we might observe the genuine emergence of novelty, *de novo* selective causation and life⁵⁵.

Conclusions

In 1912, Bertrand Russell famously wrote⁵⁸ that “*The law of causality, I believe, like much that passes muster among philosophers, is a relic of a bygone age,*” claiming causality was largely useless for the sciences. His view seemed consistent with the deterministic, block-universe picture of the physical sciences: if everything is just part of one grand,

fixed spacetime structure, then causes and effects might be no more than a convenient fiction, an artifact of our human perspective. This vision has left some of the most fascinating questions in science underexplored and unexplained. Chief among them is the emergence of complexity, including the origin of life. If the entire universe were a static block, lacking cause and effect, why would complex structures ever arise, especially self-maintaining structures like living cells? Some sort of fine-tuning mechanism for the initial state of the universe would be necessary²⁹, which is not parsimonious as it invokes extra laws (initial conditions) that are not subject to experimental explanation.

The boundary of what is possible, and can come to exist, is not fixed but expands as systems become more complex. What was once impossible becomes possible and then probable and routine once a causal mechanism is selected. No single closed algorithm defined over a predetermined alphabet or rule set can fully specify, enumerate, or predict the future set of relevant objects, even though any finite fragment of an assembly history can be simulated or analysed algorithmically after the fact. This is a physical limitation on description and prediction, unpredictability, randomness, and hypercomputation. Computation cannot be used to predict possible causal futures. This physics is testable.

The radical departure of AT from existing paradigms is the prediction of a threshold in assembly index and copy number that delineates a fundamental boundary between what structures our universe can generate spontaneously at any time, and those that can only arise due to selective construction by other objects. The threshold differs depending on the causal mechanisms defining the substrate, but a threshold always exists. Objects above the threshold, like Taxol and watches (in respective substrate-specific assembly spaces), can only exist under very specific causal circumstances that select their construction and thus cannot form outside of an evolutionary lineage.

Assembly theory formalizes how, conditioned on the structure of what we observe to exist, there is a large space of physically possible things that could also exist, but do not, because there is no causal mechanism for their formation. Thus, in open-ended evolutionary systems, the boundary of what is possible will be expanding with the amount of causation, evolving along with the assembly of objects that exist.

Our universe is large in physical volume (approximately 93 lightyears in diameter) and deep in time (approximately 13.8 billion years in clock time). Less appreciated is how our universe is much larger in possibility than in realizability. The $\sim 10^{80}$ atoms in the observable universe may sound vast, but these can only ever be used to construct a finite and relatively small number of objects. That is, the size of what is *possible* is far larger (perhaps even undefinable) than the size of what is *actual*. Living structures virtualize the possible within physical objects, by instantiating large amounts of causation in small volumes of space and time. In addition to our universe being deep in space and deep in time, we must contend with the fact that to support life and intelligence, we must live in a universe deep in possibility.

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Definitions

Object, o_i : A physical entity that is (1) countable, (2) finite, and (3) can be disassembled (or assembled) by a finite sequence of recursive steps. Measurement places fundamental limits on the observation of objects, and their decomposition into parts.

Selection: The action of causal mechanisms allowing only subsets of possible structures to persist and be observed. Unlike biological selection, which requires heredity and variation, this more general definition of selection includes biological mechanisms and those that happen outside of biology, such as the causal selective processes that led to the emergence of biological life.

Cause: Structure that appears on a minimal assembly path to an observed object. These structures are causal joins of two fragments, they are not *a priori* labelled, and their precise identity need not be known.

Causation: A material attribute revealed in the existence of objects, as encoded in a minimal assembly path.

Assembly index, a_i : The minimal number of causal joins required to realise an object under a specified set of generative rules determined from the object's intrinsic causes. This is intensive to the object.

Assembly path: A finite sequence of causal joins terminating on an observed object.

Assembly space: The physical space denoting all causal possibilities, and subject to metrological interrogation.

Virtual object: Structures that appear on a minimal assembly path and may have no autonomous existence, because there does not necessarily exist a causal mechanism that can produce identical, countable copies of these structures in high numbers.

Contingency: The dependence of an object's existence on a hierarchy of objects causally prior to its existence, where each object carries this dependence in a virtual space of finite support (a minimal assembly path).

Copy number, n_i : The countable number of each distinguishable object type, i , (defined up to limits of measurement), which provides evidence of a contingent causal chain necessary to its existence.

Measurement limit, M : The minimum copy number of a distinguishable object necessary for that object to be reliably detected and identified by a given measurement or observational apparatus.

Epistemological Threshold, a_M : A defined boundary in assembly space, set by the resolution of the measurement limit, M , where objects with a larger assembly index cannot exist and be observed in the absence of selection. This defines the boundary of the abiotic assembly space and is useful for detection of living and intelligent lineages.

Ontological Threshold, a_1 : A defined boundary in assembly space, set where the resolution of measurement is *exactly one object*, and the threshold a_M becomes an

ontological limit delineating the maximum assembly index at which an object can exist at least once in a finite physical system in the absence of selection.

Assemblage: The accumulated causal possibilities, recursively assembled to generate the set of distinguishable objects and their copies. This is a causally deep representation of matter, as it constitutes all the virtual structures necessary to the existence of the observed objects.

Assembly, A: The density of causal possibilities per observed object, taken as the ratio of the copy number in the virtual space of objects to total number of countable objects in a sample. This captures cumulative selection in accounting for both the causal depth of objects in a combinatorially explosive space (assembly index) and the persistence of the mechanisms to produce these objects (copy number)

Assembly time, a : The number of causal joins in a constructive process to produce an object.

Possibility: A causal join that can happen, or an object that can exist. These are encoded in the assembly space: possible objects or events are those that can be generated by selection.

Probability: A phenomenological means to encode the role of the environment in an object's existence, which allows quantifying the production rate or error-rate of making a specific object with a given accuracy in each existential context.

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Appendix A: Possibility and probability in assembly theory

To understand the physics underlying assembly theory (AT), it is important to make a distinction between the concepts of “probable” and “possible”. “Possible” indicates an event can happen, or an object can exist (by existing causal mechanisms as no statement can be made for causation that does not exist). Statements of possibility should *not* be confused with statements of likelihood. It is not possible to assign likelihoods to things that do not yet exist.

In AT, we do not regard statements of what is “probable” to encode *any* information about what is possible. This motivations underlying this are in contradistinction to other accounts of probability, e.g., the most common being frequentist accounts^{59–61}, propensity accounts⁶², or Bayesian accounts^{63,64}. To understand this distinction, consider a statement like “*Object A has a probability $\rho(A)$ to occur*”. Current accounts of probability will treat such a (physical or epistemological) statement as being about *A*, capturing the tendency, or belief about tendency, for *A* to occur, in many cases conflating probability with possibility. In AT, we disentangle probability from possibility: probabilistic statements about *A* are not intrinsic to *A*; instead, such

statements are about the system and environment that generated A . That is, $\rho(A)$, is a feature of a causal mechanism that can assemble A . Some causal mechanism must exist for A to be observed (this can hold for either a physical or epistemological interpretation of probability in AT). In short, in AT, we do not regard probability as saying *anything* intrinsic to the object; rather, probabilistic statements are those that encode information about what made the object. Consider the example of the ribosome, such structures possible everywhere (since we know these are possible here), but the only planet in the universe where it is probable is Earth. It is also possible that ribosomes will be probable in the future on other worlds, e.g., if Mars becomes inhabited with life from Earth; but no statement can yet be made (as of writing) about the probability of that possibility because it does not yet exist.

Possibility is encoded in the assembly space: possible objects or events are those that can be generated, as described in the definition of *assembly space* as a space of causal possibilities. Combined with the definition of an object in AT, possibility is open and undetermined, but expansion of what is possible is dependent on what objects exist. Probabilities can be assigned as a phenomenological means to encode the role of the environment of an object in that object's assembly, e.g., assigning probabilities to steps allows talking about the production rate or error-rate of making a specific object with a given accuracy (an example is in how the probability for forming a ribosome should be assigned to the cell, not the ribosome). Assigning probabilities to events or objects is only possible if those events or objects are already selected to exist, and this is not a feature of the object because it exists in a context outside the object's assembly space.

Appendix B: Derivation of assembly index threshold, a_M

An assembly theoretic question of interest is: *What is the limit on the space of possible objects with no selection?* The assembly space is a recursive, branching space, where fragments are combined to produce new structure. Being clear on the distinction

between possible and probable allows defining a threshold on what is possible in the absence of environmental or constructive selection.

As a simplification, we consider a branching process where each node has b descendants. This branching structure is a feature of the assembly space, and b allows encoding what is possible in terms of causal steps from each fragment in the space. We can also assign to each step a probability q , which is not a feature of the objects or the assembly space, but of the environmental context that might build the object (for example, q might encode the error rate in a constructor or more physically an assembler in the environment). In reality, b and q are not global parameters, but instead reflect local structure in the assembly space and of the mechanism(s) that build it, respectively. For example, b might be higher in regions of chemical space where there is a dominance of C atoms, and lower where there is a dominance of N atoms because of the possible bonds available to support causal joining in these regions. We expect q to in some cases be weakly global, e.g. in the case that some general classes of bonding mechanisms are more likely in some planetary environments due to pH, temperature etc.; in most cases q will be exceptionally local, e.g., as is the case when enzymes catalyze very specific sets of transformations to make some reactions much more likely to occur.

For purposes of illustrating the existence of a threshold, we treat these as global parameters (we will treat locality in the topology of the assembly space in future work). This simplification does not impact the conclusion of an objectively determinable boundary for the assembly index, a_M , but merely serves to elucidate its existence.

Materializing an object is the process of bringing it into existence in at least one copy. In the absence of selection, the possibility of materializing an object at a depth a is:

$$p(a) = \left(\frac{q}{b}\right)^a$$

This captures how at each step there are b new possible paths, which, if an assembler exists might be explored at a rate q . Since $b \geq 1$ (every branch has at least one descendant, and the space is open-ended), and $0 \leq q \leq 1$ (to obey the law of total probability for each branch either being realized or not). The possibility of objects will *always* decrease exponentially with a :

For $\frac{q}{b} < 1$, the probability of objects requiring long paths shrinks exponentially

For $\frac{q}{b} \rightarrow 1$, objects requiring more steps can be produced along contingent paths, indicating how selection, via the action of an assembler, can act to increase q , along specific paths by eliminating following other branches

It is not possible to assign probabilities to objects unless they are observed, thus q can only be assigned if an object already exists and there is thus an existing causal mechanism for assembling the object. $q \neq 0$ only if an object is observed (exists), The $q = 1$ case is identical to the case of equivalent exploration of everything that could be possible, that is, no selection. In the main text, we are concerned with the fundamental limits on possibility, not probability, and so we set $q = 1$, such that all branches at a given assembly time are equivalent and possible. In a combinatorial, recursively constructable space, the number of possible objects formed in successions of such events is expected to grow super exponentially, so what we present here is a very approximate argument as the space will grow much faster.

In what follows, we define $\beta = q/b$, such that a global parameterization of q is kept explicit, even if ultimately unphysical for most objects of interest. This is to allow at least some indication of how a_M can shift when physical objects become more probable because of selection, allowing the possibility for open-ended evolution and

the origin of life (and novel forms) as a continuous process (but not of course guaranteeing it as probable). In the main text, $b = 1/\beta$.

We normalize the probability over all objects by dividing by the sum over all paths/branches:

(B.1)

$$P(a) = \frac{p(a)}{\sum p(a)}$$

Such that the expected number of objects at depth a in the branching process is:

(B.2)

$$\langle n(a) \rangle = \frac{p(a)}{\sum p(a)} N_T = \frac{\beta^a}{\sum \beta^a} N_T$$

where N_T is the total number of objects over all populated branches. We note that objects either exist, or they do not, so $\langle n(a) \rangle$ cannot be < 1 (e.g., consistent with the copy number principle and establishing an ontological bound on assembly index). However, in practice most scientific instruments can detect objects if they exist in multiple copies. Thus, we define a measurement cutoff M , defined as the minimal number of copies for a scientific or observational instrument to detect the structure. For example, for mass spectrometry, $M = 10,000$ molecules.

We can define an assembly index threshold at depth a_M , where the condition at the limit of existence is met:

(B.3)

$$\langle n(a_M) \rangle = M$$

Thus, we have:

$$\langle n(a_M) \rangle = \frac{\beta^{a_M}}{\sum_1^{a_M} \beta^a} N_T = M$$

We first solve the denominator, where we note the sum runs over integer values of assembly steps, $a = \{1, \dots, a_M\}$, on the assumption that we are counting all objects formed in integer causal steps, with a minimum of one step, up to a_M steps. Noting $\beta < 1$, the sum is a geometric series and converges to:

$$\sum_1^{a_M} \beta^a = \beta (1 - \beta^{a_M}) / (1 - \beta)$$

where we have used $\sum_1^n r^k = r (1 - r^n) / (1 - r)$. Substituting into the equation for $\langle n(a_M) \rangle$ yields:

$$\langle n(a_M) \rangle = \frac{\beta^{a_M-1}}{(1 - \beta^{a_M})} (1 - \beta) N_T = M$$

We use this form to solve for a_M :

$$\begin{aligned} \beta^{a_M-1} (1 - \beta) N_T &= M - \beta^{a_M} \\ \beta^{a_M-1} (1 - \beta) N_T + \beta^{a_M} &= M \\ \beta^{a_M-1} (1 - \beta) N_T + \beta \cdot \beta^{a_M-1} &= M \\ \beta^{a_M-1} ((1 - \beta) N_T + \beta) &= M \\ \beta^{a_M-1} &= \frac{M}{(1 - \beta) N_T + \beta} \\ \ln[\beta^{a_M-1}] &= \ln \left[\frac{M}{(1 - \beta) N_T + \beta} \right] \\ (a_M - 1) \ln[\beta] &= \ln[M] - \ln[(1 - \beta) N_T + \beta] \end{aligned}$$

(B.4)

$$a_M = 1 + \frac{\ln[M] - \ln[(1 - \beta) N_T + \beta]}{\ln[\beta]}$$

Using this expression for a_M we can also revise our general expression for $\langle n(a) \rangle$. Starting from the most general form, which includes the explicit dependence on the

cutoff value of a_M we have (here we have taken the sum in B.2 up to a_M as all larger terms are zero or unobservable):

$$\langle n(a) \rangle = \frac{\beta^{a-1}}{(1 - \beta^{a_M})} (1 - \beta) N_T$$

This expression can be simplified as follows. We start with the term in the denominator:

$$\begin{aligned} \beta^{a_M} &= \beta^{1 + \frac{\ln[M] - \ln[(1-\beta) N_T + \beta]}{\ln[\beta]}} \\ &= \beta \cdot \beta^{\frac{\ln[M/(1-\beta) N_T + \beta]}{\ln[\beta]}} \end{aligned}$$

Using the property of exponentials $\beta^{\frac{\ln A}{\ln \beta}} = e^{\left(\frac{\ln A}{\ln \beta}\right) \ln \beta} = e^{\ln A} = A$ with $A = \frac{M}{(1-\beta) N_T + \beta}$ yields:

(B.5)

$$\beta^{a_M} = \frac{\beta M}{(1 - \beta) N_T + \beta}$$

then

$$\begin{aligned} 1 - \beta^{a_M} &= 1 - \frac{\beta M}{(1 - \beta) N_T + \beta} \\ &= \frac{(1 - \beta) N_T + \beta - \beta M}{(1 - \beta) N_T + \beta} \\ &= \frac{(1 - \beta) N_T + (1 - M)\beta}{(1 - \beta) N_T + \beta} \\ &= \frac{(1 - \beta) N_T + (1 - M)\beta}{(1 - \beta) N_T + \beta} \end{aligned}$$

Substituting into the equation for $\langle n(a) \rangle$ yields:

$$\begin{aligned} \langle n(a) \rangle &= \frac{\beta^{a-1} ((1 - \beta) N_T + \beta)}{(1 - \beta) N_T + (1 - M)\beta} (1 - \beta) N_T \\ &= \beta^{a-1} (1 - \beta) N_T \frac{((1 - \beta) N_T + \beta)}{(1 - \beta) N_T + (1 - M)\beta} \end{aligned}$$

This yields a final, selection free expression for copy number over abiotic possibilities:

(B.6)

$$\langle n(a) \rangle = \beta^{a-1} \left[\frac{(1-\beta) N_T + \beta}{1 + \frac{(1-M)\beta}{(1-\beta) N_T}} \right]$$

For $N_T \rightarrow 0$, both q and b also approach 0, and the limits of the equation behave as expected.

Appendix C: Derivation of abiotic assembly

We can use equation B.4. and B.6 to solve for the abiotic assembly, $A_{abiotic}$, starting from the equation for assembly, A :

$$A = \frac{1}{N_T} \sum_{i \in n_i > 1}^N n_i e^{a_i}$$

Combining all objects with the same assembly index together yields:

$$\begin{aligned} A_{abiotic} &= \sum_1^{a_M} e^a \left(\frac{\beta^{a-1} ((1-\beta) N_T + \beta)}{N_T} \right) \\ &= \sum_1^{a_M} e^a \left(\beta^{a-1} + \left(\frac{1}{N_T} - 1 \right) \beta^a \right) \\ &= \sum_1^{a_M} e^a \left(\beta^{-1} \beta^a + \left(\frac{1}{N_T} - 1 \right) \beta^a \right) \\ &= \sum_1^{a_M} e^a \beta^a \left(\beta^{-1} + \frac{1}{N_T} - 1 \right) \\ &= \left(\beta^{-1} + \frac{1}{N_T} - 1 \right) \sum_1^{a_M} e^a \beta^a \end{aligned}$$

For $e \cdot \beta < 1$ the sum converges and

(C.1)

$$A_{abiotic} = \left(\beta^{-1} + \frac{1}{N_T} - 1 \right) \frac{e \cdot \beta [e^{a_M} \beta^{a_M} - 1]}{e \cdot \beta - 1}$$

We can remove the dependency on a_M , using Eq. B.4 to yield a final expression:

$$A_{abiotic} = \left(\beta^{-1} + \frac{1}{N_T} - 1 \right) \frac{e \cdot \beta}{e \cdot \beta - 1} \left[\left(\frac{M}{(1 - \beta) N_T + \beta} \right)^2 e \cdot \beta - 1 \right]$$

We note in the discussion explaining Assembly as quantification of causation in virtual copies per realized object, we took $b \rightarrow \infty$ to represent the uncountable counterfactual possible causal joins folded into each step in the assembly space. For that limit, $\lim_{b \rightarrow \infty} A_{abiotic} \propto M^2/N_T^2$, meaning the upper limit on abiotic causation is higher for smaller systems, with potential implications for the emergence of life in smaller volumes with denser assemblages.