

The transition from constraint to regulation at the origin of life.

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*"In my opinion, the audacious attempt to reveal the formal equivalence of the ideas of biological organization and thermodynamic order ... must be judged to have failed."
— Peter Medawar, 1984, p. 226.*

Abstract: The origin of living dynamics required an evasion of second law degradation effects by maintaining critical dynamical and structural constraints, by synthesizing new components for replacement and reproduction, and regulating these interactions with respect to critical intrinsic needs and extrinsic conditions. Model systems for life's origin that focus on molecular replication (e.g. RNA-world), or co-production of components (e.g. autopoiesis), or physical containment of molecular interactions (e.g. protocells) fail to distinguish between constrained chemistry and regulated metabolism. For this reason they do not address the question of how living processes first emerge from simpler constraints on molecular interactions. We begin with a simple molecular model system consisting of coupled reciprocal catalysis and self-assembly in which one of the catalytic bi-products tends to spontaneously self-assemble into a containing shell (analogous to a viral capsule). We term this dynamical relationship *autogenesis* because it is self-reconstituting in response to degradation. Self-reconstitution (and reproduction) is made possible by the fact that each of these linked self-organizing processes generates boundary constraints that promote the perdurance of their combination and by limiting the each other. T, and because this synergy thereby becomes embodied as a persistent *rate-independent* constraint on dynamical constraint generation. It is proposed that this synergy of dynamical/structural constraint-generation is necessary and sufficient to constitute regulation as opposed to mere constraint. Two minor elaborations of this simple model system demonstrate that this simplest form of regulation can be the foundation for the evolution of two higher-order forms: cybernetic and template-based regulation. We offer this thought experiment as a plausibility proof that regulatory relationships can spontaneously emerge from physicochemical constraints.

1.1 Living thermodynamics

Living organisms are thermodynamically and biochemically open physicochemical systems. They constantly exchange matter and energy with their physicochemical environment and yet are constrained within physical boundaries and structures that are maintained through dynamic processes. The physicochemical processes that constitute living organisms tend to persist in states maintained far from thermodynamic and chemical equilibrium, whereas non-living physicochemical processes tend to spontaneously evolve toward thermodynamic and chemical equilibrium.

The physical and chemical processes comprising an organism include processes that capture and utilize energy and materials acquired from their environment and utilize these resources to perform the work necessary to remain intact and far from equilibrium. These constructive physicochemical processes are organized into complex cycles and webs of catalyzed reactions that breakdown environmentally acquired molecules and synthesize the bio-molecules that are its critical building blocks. This network of interdependent catalytic interactions enables organisms to efficiently counter the ravages of the Second Law of Thermodynamics by maximizing the probabilities of supportive reactions. This effective circularity of catalytic interactions can more generally be described as reciprocal catalysis (also termed a collectively autocatalytic set). This theoretical form of molecular dynamics has been the subject of numerous proposals suggesting that it is a defining characteristic of the living process, and a potential precursor to life (e.g. Morowitz 1992; Kauffman 2000)..

Reciprocal catalysis can also occur in non-living systems where its accelerating reaction rates ever more rapidly exports entropy into the surrounding environment at maximum rates, given the environmental boundary constraints. When these same processes are synergistically incorporated into a living system, however, the system as a whole maintains entropy export at a rate below what these processes would produce in isolation (e.g. see Deacon 2012, but see counter arguments below). This suggests that dynamical self-organization is not sufficient to account for the dynamics that constitutes a living organism. An organism's self-organizing features must in some way be regulated.

In even the simplest living organisms (excluding viruses) these capabilities involve several types of regulation. Regulation of these processes is a prerequisite to generate structures, control metabolism, determine the expression of genetic information, adapt cellular and organ system functions to changes in their immediate environments, repair and regenerate degraded and damaged structures, and orchestrate reproductive processes. Non-living open dynamical systems may also evolve from state to state within constrained domains in phase space and may even develop increasingly constrained behaviors over time, thus becoming more ordered. These are typically described as self-organizing processes.¹

¹ The term self-organization has become standard to refer to a wide range of organic and inorganic processes that tend to spontaneously increase in their local regularity in response to far-from-equilibrium input-output conditions. Many authors have argued that the term should be abandoned because of the potentially misleading

The dynamics of inorganic self-organized processes can be described as increasingly constrained over time until it reaches a stable flow where the rate of material and energy input is matched by entropy output. Thus the development of regular eddies in turbulent streams, the formation of regular convection cells in Rayleigh-Benard convection, and the increasingly regular growth of a snow crystal all exemplify a process of compounding constraints, and thus dynamical regularization, over time.

Regulation and constraint are related concepts in that regulation involves the differential imposition and removal of constraints affecting some process with respect to its development toward or away from some target state. But constraints are function-neutral restrictions on dynamical and structural variations, whereas regulation is necessarily associated with the normative organization of some process, whether determined extrinsically or intrinsically. The presence of constrained dynamics that contributes to development toward some more ordered state, as in self-organization, does not in itself constitute regulation. Regulation involves the modification of constraints with respect to changing conditions that otherwise would decrease the probability of a dynamical system achieving a given target state. The classic cybernetic examples of regulation are thermostats and guidance systems organized to use feedback to counter and minimize deviation from a set point. Such systems are designed to constrain deviation by generating work organized so that it counters each deviation. Regulation is in this sense defined with respect to a target state, which in the case of designed mechanisms serves a designed function or purpose. In other words, regulation is work performed to produce and maintain a constrained target state.

This may for example involve the generation of work to contravene a deviation as does the heating unit controlled by a thermostat, or it may involve imposing constraints on some process, as does a centrifugal governor on a steam engine. In these cases, the system is the product of a teleological (purposeful) context in which its design is determined by a preferred target state. It is also possible that an analogous mechanism could emerge by accident. For example, a geyser like the Old Faithful geyser, which erupts on a highly regular schedule, is also organized in a way that “regulates” its temperature and pressure within a constrained range via a feedback-like mechanism. This cybernetic-like behavior was of course an accident of geology. So calling this a form of “regulation” is largely analogical. But biological regulation is different. Whereas regulation of blood pressure or body temperature directly contributes to the production and persistence of the system that makes this behavior possible, neither the geyser’s regularity nor the thermostat’s maintenance of temperature helps to generate the design or persistence of the particular structures that produce these results.

connotations of this term. In the case of inorganic dissipative processes the term “self” merely signals that the source of regularity is not extrinsically imposed and the term “organization” does not imply functional organization. Ashby (1962) has suggested describing such processes and “self-simplifying,” Abel (2012) has suggested that such processes might better be termed “self-ordering,” and Deacon (2006b, 2012) describes it as morphodynamics. Here I also use the term self-regularizing as another synonym.

The appearance of corresponding component physicochemical processes in both living and non-living contexts challenges us to explain exactly what features of living organization diverges from simple self-organization and makes possible the persistence of life's far-from-equilibrium thermodynamics. The first question this poses is: How could processes that come into existence because of the way they maximize the export of entropy spontaneously give rise to a form of global dynamical organization that restrains this tendency. The second question is: To what extent does this dynamical organization also require a shift from a dependence on externally imposed constraints to one that is at least in a minimal sense is intrinsically self-regulating. In other words, must this also involve a shift in the source of form-determining influences from external to internal, and thus determine an inside/outside (self/other) distinction. This convergence of radically unprecedented thermodynamic features inverts an otherwise ubiquitous tendency characterizing the whole of the nonliving world. Yet, surprisingly, it must have involved extremely simple molecular relationships in order to have arisen spontaneously.

These requirements appear almost mutually exclusive, but together they vastly narrow the possible contexts that need to be considered to explain the origin of living thermodynamic processes. So, taken together these limiting conditions make solving the puzzle of life's origin highly counter-intuitive, theoretically informative, and yet surprisingly tractable.

1.2 The re-restated Second Law of Thermodynamics

The classic Second Law of Thermodynamics stated that isolated physical systems involving large ensembles of interacting components will spontaneously change toward a condition of maximum entropy. This classic formulation was developed and refined during the latter part of the 19th Century to apply to material-energetic interactions for isolated processes close to equilibrium. But these restrictive conditions determine a special physical context that is highly atypical and transient in the natural world. Most physical interactions occur in non-isolated (i.e. "open") physical systems that are in the process of exchanging both matter and energy with their surrounding environment. Because of this, the more typical case also includes extrinsic influences that tend to drive an open system away from equilibrium at the same time that there is a spontaneous intrinsic tendency for it to develop toward equilibrium.

Recognition of this limited application suggested to physical chemists and mathematicians during the first half of the 20th Century that it was necessary to develop a more general theory of thermodynamic change and thus a restatement of the classic Second Law that would include accounting for these relationships. Early exemplars of such a restated Second Law were suggested in the early 20th Century and more systematically formulated by Ilya Prigogine in the decades just after mid century. Whereas the special case described systems that inevitably develop toward a state of maximum system entropy, given the boundary condition (such as total dynamical energy, spatial confinement, number, and diversity of the ensemble of components), the general case focused on the rate and distribution of entropy change between a given open system

and its environment. The critical variables in such cases therefore included how a system is extrinsically perturbed with respect to its spontaneous tendency to develop toward higher intrinsic entropy and how that system's changes in turn perturb the thermodynamic state of its environment. These might be described as the system's import and export relationships, respectively, and it suggested a different relationship to the classic entropy maximization principle. Instead of a global tendency toward entropy maximization, it became clear that the import and export rates would tend to develop toward maxima given the constraints on system-system or system-environment interaction. This has often been described as the maximum entropy production principle (MEP principle). In these terms "entropy production" refers to a rate of entropy change occurring in the relationship between thermodynamically linked systems. This reformulation of the Second Law can thus be stated as:

As a thermodynamic system is “moved away from equilibrium [it] will utilize all avenues available to counter the applied gradients. As the applied gradients increase, so does the system’s ability to oppose further movement from equilibrium.” (Schneider & Kay 1994)

or more simply,

The rate at which entropy changes in the interaction between systems will tend toward a maximum (with respect to the constraints on interaction).

In this respect, the restated Second Law has become a rule of entropic interaction that in effect describes the "flow" of entropy change between systems.

The restated Second Law has been most usefully applied to the analysis of so-called dissipative physical systems, i.e. physical systems that are exporting their entropy increase to their environment. Of particular interest among dissipative systems are those described as self-organizing. This is because the restated Second Law explains how these open thermodynamic systems could locally appear to violate the spirit of the classic Second Law and increase in their orderliness and decrease in entropy.

Notably, self-organizing systems have no capacity for persistence beyond extrinsically imposed gradients and constraints. When such external dynamics cease, the self-organizing system dissipates per the second law of thermodynamics. In fact, as suggested by the MEP, self-organization is characterized by its tendency to form local order so as to dissipate the external gradient at increased rates. In this way, self-organizing system, per se, hasten their own destruction. And, as such, far from their intrinsic dynamics maintaining themselves, their intrinsic dynamics dissipate extrinsic constraints. In this respect, self-organizing systems can have no memory in of themselves.

A question that is currently a topic of debate is whether the restated Second Law is adequate (and thus sufficiently general) to provide a thermodynamic theory of living processes. To the extent that living processes are dissipative processes that can be adequately described as constellations of self-organized processes, the restated Second

Law should apply. Following this line of reasoning a number of researchers (e.g. Brookes & Wiley 1988, Schneider & Kay 1994, Swenson 1989, Salthe 2008) have argued that organisms, ecosystems, and the process of evolution all should exemplify the MEP principle.

We believe that, contrary to this view, the MEP principle is not sufficiently generalized to be able to account for organism thermodynamics. It is specifically unable to account for the capacity for organisms to maintain and reproduce their far-from-equilibrium organization in the face of both intrinsic degradation and extrinsically imposed damage or reduction of supportive resources. However, by including one more step of generalization—identifying how self-organization can produce constraints that modify dissipation boundary conditions—not only can we resolve certain conundrums concerning the special character of living processes, but we also opens the door to a physically grounded conception of function, information, and control in biology.

This amounts to a further modification of the Second Law of Thermodynamics — a re-statement — to not only include open system processes driven far from equilibrium but in addition to include open system effects that fundamentally modify the very boundary conditions that they depend on. In a trivial sense, this is the normal condition for most open system processes. Thermodynamically self-organized processes generate increasing regularity in the process of more rapidly degrading the energy gradient they depend on. The result is self-destruction of this regularity of dynamics. Including this parameter changing effect thus more accurately characterizes the time evolution of most real world self-organizing processes. But where it is a potential factor determining the evolution of dissipative processes, it is critical for even a minimal account of living thermodynamics.

1.3 The autopoietic dilemma

This property of self-organized dynamical processes poses a challenge to one of the most common characterizations of the general dynamical logic that constitutes an organism. This is because self-organization in the form of the reciprocal production of each of its components by the interactions among some or all of the others can't be denied as a critical defining feature of any living organism. This co-productive logic has long been recognized as a distinctive characteristic of life. Its first modern statement can probably be attributed to Immanuel Kant's effort to define the apparently intrinsic teleology of living beings. In his 1790 Critique of Teleological Judgment he distinguishes organisms from mere machines in terms of their reciprocal productive power as follows:

“An organized being is then not a mere machine, for that has merely motive power, but it possesses in itself formative power of a self-propagating kind which it communicates to its materials though they have it not of themselves.”

and

“... every part ... is there for the sake of the other (reciprocally as end, and at the same time, means).”

This circular component production logic has been the focus of many modern efforts to characterize what makes an organism distinctive from other forms of physico-chemical processes. In a striking parallel, the evolutionary biologist J. B. S. Haldane gave the following definition of life in 1929:

“A simple organism must consist of parts A, B, C, D, and so on, each of which can multiply only in the presence of all, or almost all, of the others.”

Probably the most commonly cited modern characterization of this co-productive characteristic of organism dynamics is Maturana and Varela's (1980) concept of autopoiesis, or "self-production." The term distinguishes the dynamics of living organisms from dynamical systems whose organization is externally imposed and thus allopoietic. An autopoietic system additionally "constitutes itself ... as a concrete unity ... by specifying the topological domain of its realization ..." So an "autopoietic machine" is one that collectively produces its material components as well as the network of relations between them that constitutes their unity in a discrete physical location. These latter properties are not attributed to any separate and distinctive mechanism over and above the closed co-production of components and yet are essential defining attributes. Indeed, this organization is described as the "fundamental variable which it maintains constant" (Maturana & Varela 1980, p. 79).²

These characterizations highlight but do not provide a mechanistic account of how this organizational unity is generated and maintained. In simple terms they need to assume some additional persisting representation of this co-productive unity that is imposed upon the collective interactions of the components. This additional factor is what regulates these processes so that their synergistic dynamical organization is maintained within narrow limits despite material replacement. So although component co-production is an important attribute of living organization. It is the maintenance of this network or dynamical relations that is what most demands an explanation.

The requirement of this additional controlling influence is well exemplified by reciprocally catalytic chemical processes. Though each molecular species comprising a

² A more explicit focus on this reciprocal organizational feature over and above component co-production is provided by Robert Rosen's (1985) conception of "relational biology." This recognizes that the material components of a living system are completely replaceable in the course of a lifetime and their forms are completely modifiable in the course of lineage evolution, yet its relational integration must persist across these changes. Rosen developed a graphic formalization of this relationship and a complex formal apparatus to deal with the distinctive self-referential structure of biological processes, though this was not applied to specific molecular or dynamic processes. Not being conversant with this formalism we will not attempt to determine whether or not it is sufficient to overcome the logic difficulties we attribute to autopoietic approaches, nor are we able to say that all the variations on the autopoiesis concept fall prey to the difficulties we describe here.

collectively autocatalytic set is a product of the interactions among other members of the set, their collective reciprocity is only an extrinsically observed descriptive property. In a solution containing such a set of catalysts diffusion processes will spontaneously undermine the process of co-production and their dynamical co-production will cease. So there is no unity intrinsic to the components or their collective co-productive relationships. Something in addition to co-production is required in order to explain living dynamics.

The most common solution offered to counter this absence of a unifying influence is to imagine enclosing a set of reciprocally catalytic molecules within a container analogous to a living cell (e.g. Maturana & Varela 1980, Thompson 2007, Kauffman & Clayton 2009). But confinement isn't unity, only proximity. Physical confinement doesn't guarantee persistent self-similarity of organization. Catalytic co-production will cease in a closed vessel. Persistence of this dynamical organization requires that new substrates are able to enter to be catalyzed and waste products are able to leave. And unless these two diffusion processes are regulated so that only appropriate molecules can enter and exit at controlled rates, consistent with the rate of catalytic production, the organization will progressively degrade. Even just the generation of new components will be problematic. Unregulated growth can only be sustained if the container itself enlarges at a correlated rate. Container components must therefore be produced at a rate that is regulated to roughly correlate with the $2/3$ power of the rate of internal component production. In addition, even if differential component production rates are controlled constant growth can only persist if non-destructive fission and re-annealing of the contained system is probable. Thus autopoiesis, at least as understood in these terms, must assume the existence of a number of the very regulatory relationships it is supposed to explain.

A final critical shortcoming of this general approach to organism dynamics is its failure to consider the thermodynamic requirements and constraints involved. As noted above (Section 1.2), organism thermodynamics necessarily diverges from both near-equilibrium thermodynamics and far-from-equilibrium self-organized thermodynamics. Together with the many above-mentioned dynamical regulation requirements that must be satisfied, the thermodynamic agnosticism of autopoietic theories renders them insufficient in both respects to account for the critical distinction between living and non-living thermodynamic systems.

1.4 The logic of biological regulation

It would thus appear that the organizational unity of even the simplest precursor to an organism requires something in addition to reciprocal generation of components in order to maintain its dynamical self-similarity across material change. This something in addition thus provides a regulatory influence over the system of interactions, stabilizing and persistently reconstituting their co-dependent organization. This additional factor, must in some sense function independently from the dynamics it regulates, otherwise it would be susceptible of modification and corruption along with this dynamics. Consequently, it must operate something like a representation or a model of this global

synergistic organization, and be able to impose the constraints implicit in this model upon the dynamical relations among system components.

Interestingly, both Rosen and Varela identify this special living logic with a symbolic formalism. Both also recognize that this formalism must have a re-entrant or recursive structure, such that it embodies what Gregory Bateson (1972) described as a logical type violation. Thus, both formalisms are essentially structured such that a term representing the whole formula is incorporated as a part of the formula describing the whole. In the same way that the classic liar's paradox leads to a non-completable analysis, this representation of the whole system's organization embodied in a component part suggests to both theorists that there is something non-reducible about this essential living logic. Rosen describes this as an "impredicate" relationship (1991) that defies analytic reduction, whereas Varela (1979) employs the logic of distinctions developed by George Spencer Brown (1972) to describe this core autopoietic property as a form of self-referential closure.

Representing the core organizational feature of a living organism as a formal rather than as a physical relationship has also been advocated in a slightly different form by the systems theorist Howard Pattee. Pattee has consistently argued for what he calls an "epistemic cut" separating the dynamical and what he calls the "symbolic" aspects of a living organism.

He argues that the persistence of dynamical self-similarity, whether in organic or inorganic systems, critically depends upon the presence of rate-independent constraints. Pattee (e.g. 1972, 1995, 2001) argues that only this segregation of dynamics and control guarantees that critical organizing constraints do not become corrupted by the ongoing dynamical processes. As noted above (Section 1.2), inorganic self-organized dissipative processes can emerge when they more rapidly degrade the gradients of energy and/or materials in far-from-equilibrium conditions. This degradation of organization is an intrinsic tendency of any self-organized process. So were the dynamical processes constituting an organism to be the sole source of regulation they would inevitably be susceptible to self-corruption. This provides another reason to hypothesize that some additional non-dynamical regulatory principle must be a fundamental attribute of any living organism and must have come into being with the emergence of the first proto-organisms.

2.1 Autogenesis and constraints on constraint-production

All naturally occurring dynamical processes are subject to physical constraints. In other words, systems inevitably change through only a subset of the possible states they could potentially realize, all things being equal. Most commonly these constraints are what might more commonly be called boundary conditions. As noted above, however, under far from equilibrium conditions new global constraints can emerge producing self-organized regularities. These are effectively internally-generated constraints, though they are generated in response to extrinsic perturbations. Constraints can be both dynamical and structural. An eddy in a stream is a dynamically generated and maintained self-

organizing process. Its form persists only so long as the flow of water remains constant and the obstruction that perturbs it from linear flow remain constant. Snow crystals provide a link between both dynamical and structural constraints. Snow crystals grow into highly regular complex hexagonally symmetric patterns as a result of a number of converging constraints. First there is the constraint of ice lattice formation which tends toward only a very few regular patterns that correlate with differences in temperature, humidity, and pressure. This allows the growing crystal to become a sort of palimpsest of the brief history of differing atmospheric conditions through which it falls. Second there is the complex thermodynamics of the phase change from vapor to solid and the heat energy this liberates into the growing crystal lattice and from there is dissipated to the surrounding air. This likely plays a role in equalizing growth and melting patterns throughout the crystal. And third, there is the structure that has been laid down at earlier stages of growth the limits the positions at which new growth is most probable. Thus, the dissipative dynamics of crystal growth leaves a structural trace that constrains each subsequent stage of growth. This allows constraints to compound on one another, and is partially responsible for the complex symmetries that result, even though interactions with new water molecules occur at random due to Brownian motion. In many respects this is a form of memory.

To demonstrate the relevance of constraint generation to living processes and their regulatory dynamics Deacon (2006, 2009, 2012) has proposed a model system consisting of two synergistically linked self-organizing processes, illustrated in Figure 1. This empirically realizable molecular complex is called an *autogen*, because of its self-generative and self-repairing properties. It consist of a collectively autocatalytic set of molecules which generate byproduct molecules that tend to self-assemble into a container, similar to a viral capsule. Because of this relationship between processes, wherever reciprocal catalysis is most rapid there will also be a growing concentration of self-assembling molecules, and so the probability of forming a self-assembling container that encloses the very catalysts that when active will tend to generate such a container will be high. So, this simple configuration results in the tendency to generate, preserve, and reconstitute three forms of reciprocal constraint.

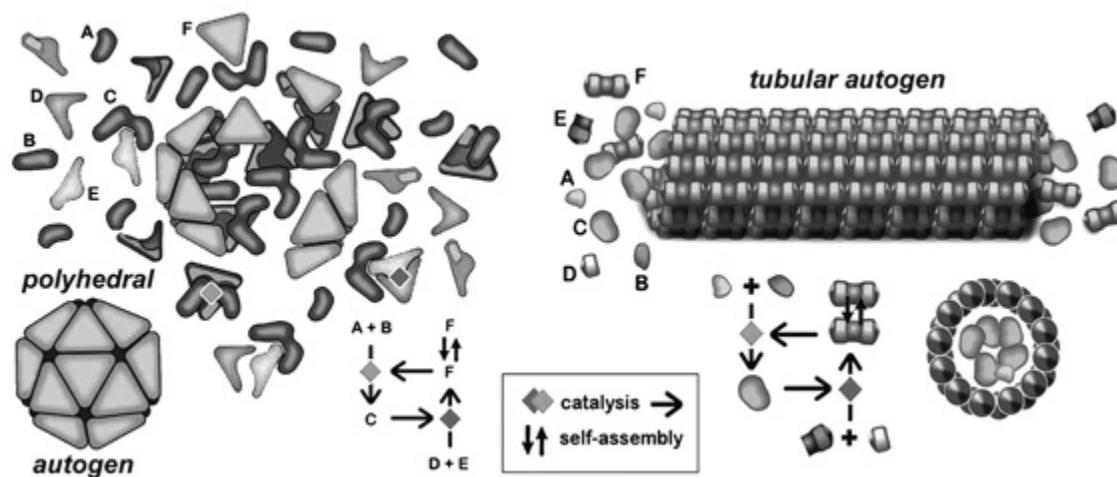


Figure 1 - Two Autogenic Systems

The first two of these constraints are physicydynamic constraints generated by “self-organizing” processes, whereas the third is a formal constraint, a consequence of formal complementarities arising out of the interactions of the first two constraint-generating processes.

The two self-organizing processes are the reciprocal autocatalytic process and the self-assembling shell formation process. Two possible variants of this relationship are illustrated in Figure 1: a polyhedral and a tubular form of autogenic process. Just as the products of each catalytic process (products C and F in Figure 1) serve as reciprocal catalyst, each for the other, one of the products (F in Figure 1) is a component of a self-assembling shell structure. It is via this process that one self-organizing process, the shell structure, limits the other process, autocatalysis, from completely dissipating the co-locality of catalytic materials and the structure necessary to maintain that locality, which is itself a product of the catalysis.

And, it is this tendency, intrinsic to the coupled fates of these two self-organizing systems, that constitutes the third constraint. This third constraint is an higher-order constraint in that it is composed of the inter-dependent dynamics of the first two. And, critically, it is the capacity for this third constraint to preserve the *potential* for further similar dynamics in a temporarily static, i.e. relative rate-independent, form that creates the foundation upon which abiogenesis, and eventually semiotics, finds a foothold.

The critical boundary constraint on reciprocal catalysis is proximity of the catalysts of the set (i.e. relatively high local concentration of these molecules) to each other. Typically, products of the reaction will tend to diffuse as soon as they are generated. However, the autogenic shell will maintain some locality, so that even when catalysis eventually reaches chemical equilibrium, both reactants and products are maintained in formal *dis*-equilibrium, relative to their surroundings. In other words, since they’ve been “captured” in a self-assembled shell (which will form most effectively in a region of high catalytic activity), spatial diffusion, which would have otherwise dispersed reactants and products (i.e. catalysts), will have been thwarted.

Conversely, the critical boundary constraint for shell self-assembly is a high concentration of a form of molecule that tends to cohere with like molecules into a shell or tube. But self-assembly itself ever more rapidly depletes the local region of these molecules as they accumulate into this structure. To effectively drive self-assembly then there needs to be a locally replenished supply of these molecules (as well as thermodynamic conditions favorable to their coherence). Local reciprocal catalytic production of these molecules provides this boundary constraint.

As a result of this reciprocity of constraint production, there is a high probability that the same boundary constraints for each will be maintained even when the complex closes and chemical dynamics ceases. This potential reciprocity of dynamical constraints will be remembered, so to speak, even though dynamical activity ceases. But if the structural

integrity of this inert molecular complex is in some way disrupted (e.g. by thermal agitation) in the presence of new catalytic substrate molecules the release of these catalysts will immediately re-initiate the process and these previously potential boundary constraints will again become dynamically expressed. Thus the integrity of the complex will be quickly reconstituted—a form of self-repair. And it is also possible that a significantly disrupted complex will reform into two or more new replicas of the original—a form of self-replication.

This tendency for an autogenic complex to reconstitute itself if disrupted means that a third higher-order constraint is generated as well. This is the constraint maintaining the complex synergistic reciprocity between the component constraint-generation processes. Indeed, this higher-order constraint is persistently present through all phases, inert and dynamical, potential and expressed. In this respect it is a formal constraint, not merely a physico-chemical dynamical constraint. This higher-order constraint is effectively a self-reconstituting boundary condition for promoting its own persistence. By reconstituting itself if disrupted this dynamical process effectively completes a work cycle which. Stuart Kauffman (2000) points out that completion of a work cycle is a necessary property of what he characterizes as autonomous agency: the “capacity to act on it’s own behalf.” This is because completion of shell closure doesn’t just reconstitute a physical structure, it comes full-circle so to speak to reconstitutes this capacity for reconstitution.

2.2 From synergistic constraint generation to regulation

We can define regulation as a behavior generated in order to constrain some dynamical system variable to a range that supports persistence or prevents degradation of that system and/or its functions.

Classic examples of regulation are negative feedback mechanisms like thermostats and autopilots. These negative feedback systems are designed to behave in a way that converges toward a predetermined target state irrespective of how they are perturbed away from this state. But cybernetic behavior does not constitute regulation in itself. In a man-made regulator this target state or range of variation is imposed by design processes that are independent of and outside of the operation of that system.

In contrast, if analogous cybernetic behavior happens to occur by chance in inorganic nature, like the maintenance of pressure and temperature in the Old Faithful geyser, we could only describe it as regulation in a metaphorical sense because achieving this cybernetic organization has nothing to do with producing or maintaining its specific organization and it has no intrinsic function (except perhaps to entertain tourists).

In recent decades roughly a thousand such feedback processes have been isolated in the human body. They are often analogized to man-made cybernetic systems. Though biologists recognize that these systems were not designed, in the sense that engineered systems are, it is commonly said that chance variation and selective preservation by natural selection has played an analogous role to purposeful design in the evolution of organism regulatory mechanisms. The problem with this seemingly reasonable analogy is

that it merely passes the buck, so to speak. This is because organism adaptation and reproduction—the critical pre-conditions for natural selection—are quintessential regulatory processes themselves. How did this regulation ultimately arise if not from prior regulation? And if inorganic processes can only be described as regulatory if serving an extrinsically imposed function how could regulatory processes ever have spontaneously emerged from inorganic processes alone?

This is where the logic of autogenesis can contribute some critical insights.

A geyser or a thermostat do not have inherent dynamics with the capacity to maintain, repair, or reproduce these same intrinsic dynamics. The constraints that constitute a geyser's oscillatory expulsions will loosen and degrade as both the heat needed to fuel them dissipates and the constrained opening is eroded by its own activity. Similarly, the thermostat, if left alone by human attention, would fall prey to entropy. Dynamics inherent within cybernetic systems must be imposed and maintained by extrinsic dynamics. In the case of the geyser such extrinsic impositions are naturally occurring terrestrial processes; whereas, for the thermostat, both its improbable structure and ultimate function are determined by human designers and users.

The intent of this paper is to present the possibility of emergence of regulation from very particular inter-dependencies among proximal constraints. The autogenic logic described above provides an exemplary system in which the co-constraints of inter-dependent self-organizing processes are sufficient to maintain, repair, and reproduce their own critical collective boundary constraints. In other words, an autogen is a model system that regulates the conditions that contribute to its own integrity by initiating dynamical activity to counter forces that would tend to disrupt this integrity. In this respect, the special synergistic reciprocity between the component constraint-generating processes constitutes a minimal form of regulation at a higher level. In effect, it marks the emergence of the regulation of "self" in a literal physical sense. This self-regulation organizes the component physico-chemical constraint-generating processes that constitute it, but is not a physico-chemical constraint in itself.

This satisfies a requirement that Howard Pattee (discussed above) repeatedly argued must be a fundamental feature of life: the regulation of organism dynamics by a rate-independent constraint (which he characterizes as a "symbol," presumably intending to appeal to some sort of generic semiotic element). As noted above, the higher-order constraint on the relationship between the component constraint-generating processes of the autogen persists whether or not the system is inert or dynamically reconstituting itself. This regulatory influence persists independent of the autogen's dynamical state or the shuffling of its specific individual molecular constituents, and is even capable of being reproduced. But this autogenic form of self-regulation is not an extrinsically imposed semiotic influence. It is literally constituted by the formal relationships between dynamical processes. In this respect, there is no "epistemic cut" between physico-chemical dynamics and the formal source of regulation, as Pattee often referred to this dichotomy. And yet this hierarchic distinction between component constraint-generation processes and the formal synergy-maintaining rate-independent constraint embodied by

them effectively creates an intrinsic semiotic relationship. Whereas Pattee's exemplar of a rate-independent semiotic constraint is the structure of a DNA molecule and the way this indirectly constrains the molecular dynamics of a cell.

One obvious clue that this form of organization crosses the boundary from constraint to regulation and out of the domain of merely physico-chemical processes is that regulation can succeed or fail. Physico-chemical constraints are present or absent. Certain processes will thus either occur or not as a result. Constraints per se, can neither fail nor succeed. They merely exist, because, for continuously dynamic inorganic processes there is no "set point" or preferred state other than equilibrium.

The autogen, however, illustrates just such a "set point" which simultaneously embodies the capacity to persist at that set point and return to it when perturbed. This set point is effectively its completed inert form. An autogen can persist in this inert state indefinitely, unless sufficiently perturbed, at which time its preserved reconstitutive potential will tend to return it to that state preserving this potential. This set point can in this way be "remembered" even when conditions are not conducive to its dynamical reconstitution. So an autogen is like a cybernetic regulator in this one respect: there is a target state that defines the end or the function that is regulated. Also analogous to a cybernetic regulator, an autogen's set point is maintained irrespective of the system's dynamical state. But unlike a designed cybernetic system, if an autogen is dissociated in a context lacking sufficient substrates or energy to drive its catalytic processes, this self-regulatory capacity will fail to be regenerated. Or if there has been an accidental molecular substitution in one of the component processes the self-regulatory capacity may be degraded. Thus an autogenic process is regulatory in a more complex self-directed way than is a designed cybernetic regulator. Its regulatory function is intrinsic to its very constitution.

This hierarchically organized constraint relationships can thus be considered to offer a plausibility proof for the emergence of telos (a form of final causality) from mere physico-dynamic constraints (efficient causality). Regulation has no meaning without the existence of telos, and telos has no meaning without the existence of a "self", for which one end should be preferred over another. It is the self that persists or not depending on some outcome. In contrast, in the non-living world outcomes are irrelevant to any given dissipative physico-dynamical process. All mere physico-dynamical constraints necessarily must dissipate per the second law of thermodynamics. This fate, however, is not inevitable for living organisms whose lineages could potentially propagate their particular kind of regulation of constraints indefinitely, because they are effectively rate-independent.

Although, the origins of life might conceivably have involved a very different chemical constitution, it would be our contention that it necessarily must have involved an analogous autogenic logic. It requires the emergence of a higher-order self-regulation out of the synergy of lower-order constraint generation processes. This requirement would rule out scenarios involving simple molecular replication or even simple contained self-replication of RNA molecules (versions of RNA World) or autocatalytic molecules (versions of autopoiesis), because there is no explicit regulation of system integrity

involved. But for the same reason that this is a plausibility proof for the emergence of self-regulation and end-directed dynamics, it is also a plausibility proof for abiogenesis.

Of course, as with life in general, there will inevitably be changes in the environment that tend to undermine the preservation of any lineage with these characteristics. The capacity to reproduce and therefore provide a sort of lineage memory of this regulatory logic is the necessary basis for evolvability and the ground with respect to which new adaptations can be acquired. A core dynamic that self-regulates the processes that work against degradation becomes a sort of magnet for any additional variants that contribute to this self-maintaining capacity. This minimal form of evolvability despite the lack of specific molecular replication and inheritance mechanisms (but see below) thereby also provides the overarching dynamic that makes possible the evolution of higher-order more complex forms of regulation, as will be discussed below.

3.1 Conditional autogenesis: The emergence of cybernetic control

Given the self-regulating autogenic system described in section 2, the basis for a form of lineage evolution is established with the possibility of diverse variant forms. On one hand, this population will embody a kind of formal memory of what kinds of higher-order synergistic constraints have sustained individuals in past environments. On the other hand, each generation provides an opportunity for some small degree of variation to accumulate distinguishing individuals and their progeny. This might for example arise to the periodic incorporation of different molecules into the complex during a dynamical closure phase. To the extent that these new molecules insinuates itself into one of the component processes and interacts favorably it may itself become incorporated in the global autogenic dynamic. So long as the core self-regulatory capacity remains intact across future replications this new variant will persist as well. This is the basis upon which higher-order complex forms of regulation can evolve.

Consider one such possible advantageous variation: an autogen in which a shell molecule is structured so that catalytic substrate molecules will tend to stick to it. If as the number of bound substrates increases the shell become increasingly unstable an adaptive consequence will follow. In general, as reactants are consumed from the environment during autogen formation, the local environment will become progressively less supportive. If an autogen achieves its inert form, however, more substrates will likely have a chance to diffuse out of this locale and the inert autogen will also tend to diffuse to other locales as well. The probability that a simple autogen will be disrupted and caused to reinitiate dynamical self-reconstitution is entirely independent of whether substrates are or are not present in the environment at that time. But an autogen with a surface that is sensitive to the presence and concentration of substrates (see Figure 2A) will be less likely to get disrupted in the absence of environmental substrates and more likely to do so in their presence. This context-sensitive biasing of the constraint on shell fragility can thus serve as an adaptation which improves the probability of successful reproduction. Consequently, an autogen lineage with this added capacity will tend to out reproduce an autogen lineage that is insensitive to this relevant environmental factor.

A correlation between structural fragility of a molecular structure and the presence of a particular molecule in its environment would be irrelevant in the absence of the autogenic capacity. In the context of a molecular system embodying this autogenic capacity, however, this correlation becomes a higher-order form of regulation. The autogenic complex now includes something more than just the regulation of the synergy between constraint-generation processes. It also regulates an additional synergistic relationship between the activation of these processes and an environment that promotes their function in preserving the system's capacities. The extent of surface binding becomes an *indication* of the favorable or unfavorable state of the environment for promoting replication. In other words, it is information *about* the environment for a self-regulating system that depend on the environment. One might even be justified in claiming that this second level of self-regulatory dynamics *interprets* this change in the environment by virtue of its self-serving change in responsiveness.

This is analogous to cybernetic regulation to the extent that it is differentially activated with respect to specific variations of a selected feature of its environment. This correlation between changing context and autogenic dynamics is deviation-minimizing with respect to reproductive success. The self-regulation of simple autogenesis is only responsive to changes in structural integrity. This augmentation of self-regulation is a regulation of this regulation of integrity with respect to the environment. This is what warrants describing it as second order regulation.

This conditionality is a “decision” node, whereby one state is non-linearly changed to another state in such a way that fitness and the capacity for particular constraints to persist is significantly increased. This constitutes not only regulation of the self by the self, but regulation of self-regulation with respect to the value of a particular environmental variable. This developmental step moves information, memory, and regulation closer to biological control.

The capacity for autogenesis to itself become subject to regulation illustrates the fact that intrinsic forms of cybernetic regulation can emerge spontaneously, but only as dependent on this more fundamental form of self-regulation. Autogenic dynamics provides a bottom platform upon which secondary forms of regulation can be built.

This suggests a bold two-part hypothesis: 1. Autonomous regulation (i.e. regulation not imposed from outside the system) can only emerge in systems that embody a self-regulatory integrity-maintaining capacity as their core dynamical tendency; and 2. this capacity can only emerge spontaneously from the reciprocal synergy of constraint-generating processes that are logically analogous to autogenesis.

3.2 Template regulated autogenesis: Offloading semiotic control

We are now in a position to re-address the question of the emergence of semiotic control, such as proposed by Pattee as the defining feature of organism dynamics. We have shown (above) that the self-regulation that characterizes autogenesis is itself a formal rate-independent constraint that can thereby be maintained and reproduced irrespective of the

current presence or absence of dynamics. But this form of higher-order constraint on self-integrity is embodied holistically, so to speak, in the distributed relationships between component processes. In all living organisms, and even viruses, the critical rate-independent self-determining constraints are embodied in specialized molecules: DNA and RNA. This poses the problem of explaining how information *about* the self-regulating dynamics of an organism and critical to its generation can become off-loaded onto the physical structure of a specialized molecule.

Before presenting a scenario demonstrating how this too can in principle be explained as an elaboration of autogenesis we need to provide a caveat. More than the previous conceptual models of autogenesis this scenario will require us to merely imagine the plausibility of some novel molecular chemistry. Though not totally implausible or magical, these chemical leaps of faith help to making this “just-so” scenario more heuristically accessible. However, the absence of specific chemistry does not undermine the validity of the general principle we outline. Our point is not to offer this as a proposal for the evolutionary origins of these complex molecules, but rather to demonstrate the general principle by which the sort of holistically embodied constraints of an autogenic process can become offloaded to a component molecular structure. Indeed, it is likely that the first molecular template that took on this function in the early stages of the precursors to living organisms was something quite unlike the polynucleotides that serve this function today. We leave the search for these precursors to future generations, and here merely intend to exemplify a general principle.

As a preface to this scenario consider a curious coincidence exemplified by two core features of the molecular metabolism of living cells. The first is that the energetic functions of cell metabolism depend on one general class of energy-ferrying molecules: nucleotides like cAMP, ATP, GDP and their relatives. The second is that the information-bearing molecules within living cells, such as DNA and RNA are also composed of nucleotide residues strung together as polymers. The scenario we propose assumes that the energetic function of nucleotides preceded the evolution of the information template function of nucleotide polymers.

We begin this fanciful scenario by postulating the evolution of a molecular mechanism for the autogenic synthesis of diverse nucleotides, and an autogenic process in which these nucleotides serve to capture environmentally energetic free phosphates and use this energy to drive catalytic activity (Figure 2B). This mechanism for energetically driving the catalysis could provide both more rapid autogen reconstitution and produce molecular forms that are otherwise energetically very improbable, and in this way could provide a reproductive and thus evolutionary advantage for this form of autogen. In the inert state, however, nucleotide phosphate functions would be irrelevant or even potentially damaging. But as autogen closure shuts down catalysis it might also facilitate polymerization of the free nucleotides (e.g. by linearization effects and the exclusion of water) into a randomly ordered polymer analogous to DNA or RNA (Figure 2C). To the extent that the sequence of nucleotides provides a three-dimensional structure on which catalysts can align via hydrogen bonding there it will result in the differential proximity of different catalysts in a way that correlates with nucleotide order (Figure 2D). This

provides a sort of template/ The differential proximity of catalysts could potentially play a role in their likelihood of interacting with one another, because that those nearby each other will be more likely to be released from this polymer chain in close temporal succession. This means that template structure can provide a biasing constraint on catalytic interactions. With only a very few catalysts this would probably not make any significant difference in autogen reconstitution, but as the number of catalysts increases in evolution selective biasing of molecular interaction will become increasingly important. The more interacting types of molecules the more possibilities for molecular interaction that are not conducive to autogenic reconstitution. The “combinatorial explosion” of these possible compromising reactions will thus pose a severe complexity limit on unregulated autogenic systems. Template biasing will thus be a critical step necessary to enable the evolution of autogenic complexity.

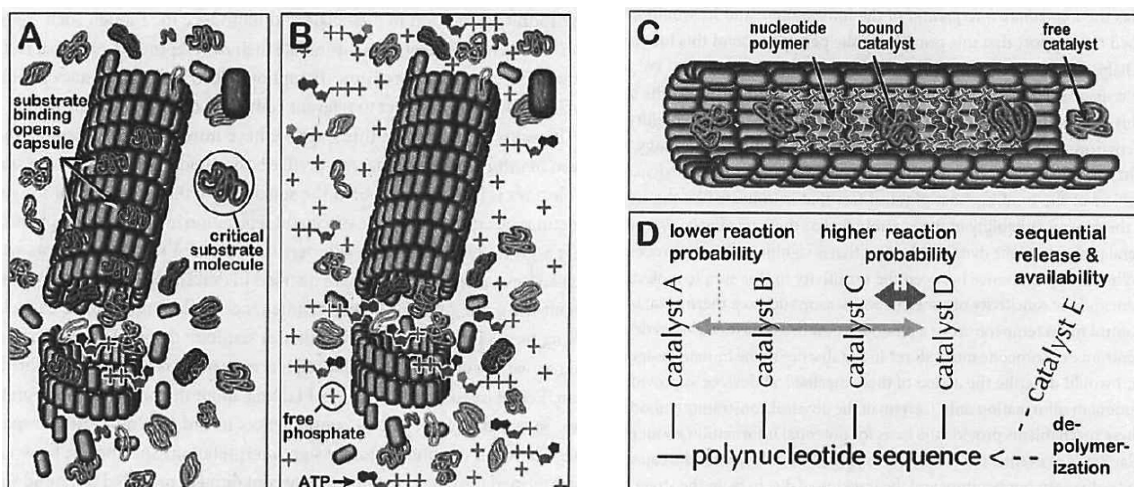


Figure 2. A. A tubular autogen with a shell that is made increasingly fragile due to the binding of catalytic substrates. B. A tubular autogen that uses nucleotides to capture and deliver energy in the form of phosphates.

C. A tubular autogen with catalysts binding to and aligning on a polynucleotide. D. Depiction of how proximity of bound catalysts on a randomly structured polynucleotide might bias catalyst interaction.

For this template scenario to work two additional conditions need to be met: the template needs to be replicated in daughter autogens and there needs to be variation in the templates that are replicated (analogous to DNA point mutations). Of course, these assumptions are also required for any polynucleotide replication theory of life’s origins. What differs in this autogenic scenario, however, is that this provides the conditions that will enable template sequence variants to be selectively favored or eliminated with respect to their correlation with more or less optimal patterns of molecular interaction for autogen reproduction. Though nucleotide sequence order may begin in a random state, selection on the relative efficiency of reproduction due to minimization of costly side reactions in a population of autogens will progressively bring about convergence on a

sequence order that maximizes molecular interaction patterns for their reproductive effect. The result is a template that embodies in its physical structure a representation of the specific dynamical organization that constitutes autogenic identity.

This somewhat fanciful scenario is a stand-in for any template evolution process that could provide some degree of biasing of molecular interactions in an autogenic context. Though quite primitive in comparison with DNA determination of the amino acid sequence constituting a protein, it nevertheless demonstrates how complex global regulation of a many component molecular network of interactions can come to be controlled by the structure of a molecule. This has many advantages over the holistically distributed global self-regulation of the simple autogenic process, though it ultimately derives this functional capability from this more basic form of regulation. The resulting template molecule has effectively offloaded constraints that previously were necessarily embodied in each of the component molecules themselves, and in this way reduces constraints on what specific molecular details are required to make autogenesis possible. Moreover, incidental modifications of template structure can now provide an indirect means for alternative catalytic interaction patterns to be generated and tested by natural selection.

The general principle that these scenarios illustrate is that the ultimate foundation of autonomous regulation is dynamical even though the locus of regulation is a rate-independent relationship. This also provides a hint about how we can avoid the methodological cartesianism of postulating an epistemic cut between semiotic regulation on the one hand and physico-chemical dynamics on the other. Regulation is not extrinsic to physics, it emerges from it, and yet it stands apart from it as well.

4 Conclusions

In this paper we have provided a model of the kind of system (an autogen) that demonstrates how merely physically and/or chemically constrained processes can spontaneously rise to the level of genuine regulation.

An autogen is composed of two or more self-organizing (i.e. self-regularizing) processes that interact in precisely such a way that each generates the boundary constraints that facilitate the development of the other while at the same time preventing the thermodynamic tendency of each to reach its natural state of maximum entropy. This mutual promotion and prevention of each process by the other via interlocking synergistic constraints, creates a uniquely integrated systemic unit. Their synergy constitutes a higher-order constraint on relations between constraint-generation processes. In effect this renders these otherwise unrelated self-organizing processes into a single self-maintaining, self-regenerating, even self-reproducing system.

All dynamical processes, whether close to or far from equilibrium, are structured so that they dissipate any labile gradients and promote development toward ever-higher global states of entropy. Self-organizing processes are special cases that increase the rate of gradient dissipation by developing increasingly more direct and therefore regular pathways for gradient reduction to occur. This local regularization is the most effective way to undermine the very conditions that produces it. In contrast, the unique interfolding combination of self-organizing dynamics that constitutes autogenesis accomplishes the

opposite. It is organized in such a way that it preserves and reconstitutes the conditions that support it, even in the face of intrinsic and extrinsic influences that tend to undermine it.

Autogenesis is thus regulation of the reciprocity of the physico-chemical constraints that are required to protect this same regulatory capacity against degradation. It is this anti-entropic self-rectifying character that warrants describing its constituent processes as functions and calling this higher-order constraint a form of intrinsic regulation. It is the regulation of the conditions that make this regulation possible and likely to persist. Because this regulates system integrity and unity it also constitutes a form of autonomous self, organized to support its own continued existence. This self is the rate-independent substrate-neutral constraint on constraints that persists irrespective of the system's changing dynamical status.

Finally, in addition to demonstrating the physico-chemical basis of intrinsic regulation, we believe that autogenesis is the platform from which (and upon which) all secondary forms of regulation can arise. This is exemplified by demonstrating how it provides the necessary scaffolding for two higher-order forms of regulation, which we describe as cybernetic and template-based regulation, respectively. Though these conclusions are derived from conceptual models not organisms, these models are based on well-understood physico-chemical principles, which makes them empirically testable. In this respect, if such systems are even remotely realistic (and even if they have nothing to do with the origins of life as we know it), they provide a "proof of principle" that true regulation can emerge spontaneously from physico-chemical constraints.

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