



# Energy-driven competitive mechanism of entropy change and its applications

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## Abstract:

The origin of life and its evolving dynamics is tightly related to molecular dynamics of initially ‘small’ molecules in the presence of permanent energy source. The point of this note is to discuss the mechanisms of life dynamics, including the entropy-related explanations and their limits. The statistical context introduces many ‘particles’ and their degrees of freedom (DoFs), and in an equilibrium energy is equi-partitioned and entropy is maximal. Meanwhile, the real ‘particles’ have an internal structure with discrete energy levels and related states. So, the excitation of molecules and their elevated reactivities drive the directed attachments/growth which increases the number of DoFs, an option used to be beyond the statistical context. A detailed approach indicates to the preferential selection of the larger particles which better *reuse* the captured energy by spreading it over the available DoFs. The smaller ones lose energy and get used as building components. The net result is an energy-driven non-stop competitive growth of increasingly larger particles - until the energy source and the building components are available. This way the energy loss due to dissipation gets minimal and the energy reuse gets maximal. The growth itself is a ‘side effect’ of the primary process of *competitive spreading* of incoming energy into increasingly larger number of DoFs.

**Keywords:** molecular dynamics; excited states; lifetimes; history trait; maximal energy reuse; permanent non-equilibrium; molecular search; entropy changes; von Neumann entropy; direct evolution

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## 1. Introduction

### 1.1. Physics of Darwin selection and entropy changes.

Observationally, life is a non-stop growth of living matter with steady increase of its complexity. Often this dynamics is related to the entropy change. A Darwin’s concept of evolution by selection of the fittest species by environment was an important step in understanding of observable species dynamics. Then Boltzmann, Lotka, Guilleminot, and others have pointed out (see review in [1,2]) the relationship between the energy use

for survival and the *selection* capability. Lotka [1,2] even considered the Darwin selection principle as a physical principle and has pointed out that the ‘winner is the best user of energy’ vs. the best fitter.

Entropy is a concept used to describe a state of classical (such as an ideal gas) system in an equilibrium, where the entropy is maximal and energy is equi-partitioned over all available degrees of freedom (DoFs). Meanwhile, the 1st and 2nd laws say what *can't be* - they say nothing about the *direction where* the system will go [1]. This is the reason for special place of the Lottka' Selection Principle which indicates *where* a system go - to maximize the energy flux rate [1,2]. The big challenge though still remains - *why it happens?* “Maximum energy flux rate” is a powerful hypothesis, which still needs to be explained. The proposed mechanism of competitive sampling is a step in this direction.

The analysis of entropy and its changes in various environments and under various ‘driving forces’ may be indicative in terms of what happens with the organization of the system in question. In fact, entropy is designed to describe the degree of spatial and temporal *organization* of a real-world systems. The entropy used to be applied to classical (vs quantum) systems, though its in-depth interpretations go beyond the standard indicators of order and/or disorder and allow for new interesting applications. However, in the life dynamics applications, classical (thermodynamic) entropy needs to be used cautiously since living matter has peculiar properties (such as growth, spatial coherence, history trait, etc) which require more detailed quantum description. Specifically, the quantum (von Neumann) entropy  $S_q$  is based on using quantum density matrix  $\rho$  and is its simple function that includes all the quantum states of a molecule/species and their populations (densities). Under certain assumptions (when the quantum properties are basically neglected), the  $S_q(\rho)$  becomes the classical Gibbs entropy.

Following the ‘physical’ perspective of energy-driven evolution[1,2], we look into physical dynamics of a molecular system in the presence of permanent energy source and ‘building materials’. For that relatively little-studied case, our analysis points to emergence of a new kind of *guided* evolutionary dynamics, a *non-stop competitive growth* of molecular species. This dynamics is unusual as it has a *history trait*, a non-stop growth in time. The history trait makes life dynamics quite unusual from view point of physics and thermodynamics and needs an in-depth analysis. Analyzing its mechanism we find that it includes the energy-driven molecular *sampling* and *testing* processes aimed to maximize the energy reuse rate. This dynamics can be seen as a guided search in the sampling space. The guidance is due to the universal trend to spread available energy over increasingly larger number of degrees of freedom(DoFs), a feature often interpreted in terms of entropy increase. In turn, such a trend is based on the universal *connectivity* or *coupling* between the units of real-world matter - atoms and molecules via their various types of bonding mediated by electronic states.

The growth increases the number of DoFs making it easier for energy to spread which increases entropy. However, due to permanency of (energy) gradients in the biosphere and unlimited availability of ‘materials’, the total equipartition may take a ‘long’ time - 4.5 Byr and still counting. Meanwhile, for a separate species and in an ‘in-between’ time, the energy gradient is still in the process of spreading and the species is steadily away from equilibrium, so the entropy gets steadily decreased. So, it seems that the concepts of equilibrium and classical (thermodynamic) entropy are hardly directly applicable to a living matter and to its separate species.

### 1.2. A history trait in the molecular dynamics and entropy connection.

The history trait, a quite uncommon feature in physics, makes the state of a molecular system *chronological*, that is, *emergent*, unfolding as a sequence of steps/events in time. J. Bernal [3] explains it as follows: "I had a very interesting discussion on this point with Einstein in Princeton in 1946, from which it appeared to me that essential clue was that life involved another element, logically differing from those occurring in physics at that time, by no means a mystical one, but an element of *history*. The phenomena of biology must be, as we say, contingent on events. In consequence, the unity of life is part of the history of life and, consequently, is

involved in its origin".

The electronic states used to be but indirectly involved in discussions of life and its origin (say, in plant photosynthesis). Meanwhile, J. Bernal also envisioned and pointed to a critical role of electronic states in life dynamics, in particular, to their potential of interactive self-realization. He wrote: “Life is a partial, continuous, progressive, multiform and conditionally interactive self-realization of the potentialities of atomic electron states”. ([3], Preface, p. xv). We’ll see that indeed the *excited* electronic states due to their *elevated reactivity* may play critical role in mechanisms of life.

Though in molecular physics the history trait is not a common concept, some processes, for example, the crystal and polymer growth may have history-dependent dynamics such as saturation effects, time-sensitive re-crystallization, and time-dependence on conditions of growth initiation, heating dynamics, etc. All these factors impact the temporal dynamics of crystal growth, polymerization, and proteins behavior (including the protein memory effects). In quantum physics the history trait is always present - as a phase memory of an (electronic) state, as an energy level *degeneracy* to be removed in interactions, and other memory-related phenomena [4,5].

In the biological context, the growth and differentiation are most significant examples of history trait. *Growth* is a well-known example of species changes in time. The *differentiation* is its another side, an *emerging* history trait. Both serve to maximize the primary function, an energy reuse, by growing the hierarchy of internal membranes and compartments to minimize energy dissipation. Its unavoidable ‘side effect’ is that in time, gradually the created hierarchy of barriers (to energy losses) slows down sampling dynamics and energy reuse until it eventually stops. We hypothesize that such universal differentiation dynamics is related to ageing and death in plants and animals. We look into details and discuss techniques how to delay the ageing dynamics by the man-enhanced sampling which improves the energy reuse.

## 2. The proposed concept and its scope: results and discussion

### 2.1. Reactivity of molecules, competition, and its driving force.

The *key idea* is that the *excited* electronic states of molecular species and, in particular, the *difference* in their *reactivity* and *lifetimes* create the *competition* between them for partners to attach. This competition results in predominance of certain excited molecules which better reuse the excitation energy comparing with other excited species that lose it by re-emission or otherwise. The longest-living species have a better chance to find a matched partner while the shorter-living ones are less likely to find a partner, end up losing energy and become a growth ‘material’. Indeed, the largest ones better reuse energy as they have more degrees of freedom(DoFs). This non-stop competition can also be seen as a *search* in the configuration space for the best energy reuser(s).

We investigate the mechanism of this non-stop competitive growth and the *emergence* of species with an increasingly better energy reuse rate, that is, the mechanism of maximization of energy reuse rate (or minimize energy dissipation rate). We identify details of search/competition mechanism, discuss options to guide it, and use it in other synthesis and growth applications. As far as we know, this type of non-stop (evolving) molecular growth by molecular competition/search was not a subject of any in-depth investigation.

### 2.2. Mechanism of maximization of energy reuse rate.

Early [4] we have discovered uncommon molecular dynamics - a *non-stop* growth of molecular species provided that the energy source and growth material are available. In the growth process, the *larger* samples, having more degrees of freedom(DoFs), better reuse energy by spreading it over available DoFs. They stay longer and have the energy and reactivity to keep on the growth. Smaller shorter-living species lose energy and become a ground-state (passive) building material for attachments. The details of this mechanism can be

found in [4,5]. The non-stop sampling and physical *testing* of various configurations against their energy reuse rate is a critical feature of proposed mechanism. Meanwhile, the non-stop growth of the excited/reactive species is actually its ‘side effect’, a tool to maximize the number of DoFs.

The species lifetime is also critical: the longer-living species have a better chance to attach/grow and thus reinforce their energy reuse capability. And the process goes on and on while energy and materials are available. The lifetime of the excited state of a species is *unique* characteristics. The range of the lifetimes may be quite wide, in some cases many orders of magnitudes [4,5]. Due to the wide spectrum of the lifetimes and the variety of the attachment partners, the search for a partner (and so growth) used to be highly successful. Provided that energy and material supply is available, the process is massively parallel in space and in time.

Even if a *single* molecule gets excited by an energy pulse, it may relax with re-emission some energy, splitting off the fragments, and moving energy into internal vibrational and rotational degrees DoFs. A *single* powerful enough pulse of energy may launch a sequence of relaxation processes so that in a while a set of newly grown particles will be generated with some species grown enough to have certain *distinctive* features such as a *history trait*. A *permanent* source of energy launches a *non-stop* molecular dynamics of the *excited* species with the sampling and testing features so that in a while the search-capable ‘intelligent’ species may emerge. The intelligence though is a ‘side effect’ of the *primary* process aimed to maximize the energy reuse rate, a means to accelerate it. In a while, even a single big enough species may develop search capabilities if an energy source is available.

### 2.3. Built-in differentiation, its limits and its unforeseen side effects.

One of implications of energy reuse maximization [4] is a ‘built-in’ *differentiation* and its structural features and dynamics. To increase the energy reuse rate, the competitive molecular search creates the architecture and structural features which physically minimize energy losses - the hierarchy of membranes, shells, internal compartments, skins, etc. Thus, the growth and *differentiation* is a ‘tool’ of maximization of energy reuse rate. While discussing the basic competitive growth mechanism, we have found [4] an alarming side effect of the accelerated growth. Indeed, the maximization of energy reuse rate requires the ever increasing hierarchical differentiation by creating membranes and compartments which minimize energy dissipation. This in turn creates the increasing barriers and other obstacles for energy spreading and reuse which we link to an unavoidable ageing and finally death.

Meanwhile, the differentiated growth has a limit. Indeed, at all hierarchical levels the membranes, shells, and compartments obstruct the sampling and competitive energy reuse which gradually slowdown the growth itself until total stoppage. We hypothesize that this is the cause for ageing and finally death of a species. So, initially the differentiation enhances energy reuse, but the advanced differentiation slow it down up to total stoppage. This non-stop dynamics needs an in-depth analysis to find options to slow it down by various *re-differentiation* techniques, including the use of stem (undifferentiated) cells as well as more efficient ‘dry’ (vs. wet) techniques with flexible control options.

### 2.4. Molecular search and intelligence.

*Entropy perspective.* Following Lotka, we tend to view this universal energy-driven molecular dynamics as a mechanism of Darwinian selection which Lotka considered as a physical principle [1,2]. Basically, it is a non-stop capture and reuse of available energy by the global multi-species molecular system, by the biosphere. A common vision of Darwinian selection in terms of separate species and their evolution is certainly useful but needs an in-depth understanding of its mechanism. This would help better understand the nature of diseases and approaches to their effective curing. The key dynamics is a *direct* molecular sampling

and testing the samples against energy reuse capability that leaves only the energy-rich (metastable) molecular species with the most efficient spreading of energy over available DoFs. Species less efficient in spreading energy lose it and become a building material. The dominance of the largest and most complex species is a result of competitive *search* in the samples space.

From this perspective, the global molecular system is in the non-stop increasingly efficient energy reuse mode capturing energy into excited state(s) and redistributing/spreading it into all available DoFs. Such a spreading of energy into available DoFs may be interpreted as an entropy increase. However, this dynamics actually occurs in a single molecule or species, where the entropy concept is hardly applicable directly. However, when applied to the global molecular system (such as biosphere) it seems it is in a *permanent non-equilibrium state*, which may be interpreted as a permanent entropy decrease. From von Neumann (quantum) entropy [12] perspective, the biosphere is in the non-stop process of spreading incoming (e.g., solar) energy into the emergent - growing by competitive energy reuse - substrate. Its ever increasing complexity is simply a side effect of maximal energy reuse. This ‘active’ process likely can be described properly in terms of changes of von Neumann entropy, an interesting option for future research.

The proposed energy reuse dynamics has some features of a *hypercycle* [9], a model of the [chemical origin of life](#). Indeed, in the model the ‘self-replicative’ units are connected in a cyclic, [autocatalytic](#) manner. From random distributions of chemicals, the hypercycle model seeks to find and grow sets of self-reinforcing loops. This model is still too formal though its logic seems to be very relevant.

The energy-driven energy reuse dynamics makes this process *directed* and ‘intelligent’. The direction gets determined by the competition to maximize energy reuse. The intelligence gets expressed via *search-capable* molecular dynamics which emerges at molecular, actually, at electronic level due to the critical dependence of the outcome on the electronic states and the lifetimes of the species involved. The search/competition is massively-parallel in space and in time. This is how nature develops and expresses its intelligence, how it ‘computes’. Numerical computing including an abstract concept of a *number* was designed to count and handle separate elements of reality - seemingly a purely man-made one. However, it is also can be seen as a result of the molecular search and intelligence by nature but in the form of man. The proposed dynamics has very much to do with the developed in recent years ‘direct evolution’ methods [6,7,8].

### 2.5. Search dynamics: performance, limits, and the guidance options

The emergence of search-capable molecular dynamics seems to be a *universal* event on any planet since it requires only an energy source and the building materials. If so, it would be of interest to ‘detach’ this molecular search capability, to identify its external control parameters/options, and to try to use it in other conditions and environments. This is a promising area of in-depth research and development. For example, when it comes to molecular computing, one approach under active research currently [5] is to simulate common computational operations using molecular movements, transformations, etc. We are interested more in possible *direct* use of molecular search in other molecular processes and less in simulation of numerical computations. This will be a subject of a separate analysis.

### 2.6. Emergence of a genetic storage - a growth acceleration capability.

Another implication of energy reuse maximization [4], is the energy-driven emergence of a species’ internal *control capabilities* aimed at acceleration of growth and so energy reuse rate. An ‘old’ way to maximize energy reuse is by a ‘regular’ growth, when an excited/reactive molecular species finds a matched partner and attaches it - each time beginning the search from scratch. Meanwhile, the *competitive* sampling tries continuously to find options to *accelerate* the growth, that is the new DoFs, to maximize the energy reuse rate. The acceleration can be achieved by enhancement the “from-scratch” trial-and-error responses with the ‘tested’ and stored multi-step ‘programs’ to control responses thus *reusing* already available control options to respond. The emergence of storage capability (‘genetic’ memory) occurs in parallel as a component of the

same energy reuse maximization process. The *soft* substrates are necessary to store the sequences. In the organic world, the best candidates for such a function are the 3D H-bonded lattices, a typical part of the organic substrate including DNA/RNA and many other biomolecules. Meanwhile, the DNA/RNA architecture has the most dense 3D H-atom lattice with programmable/soft H atoms in the H-bonds between the nucleotide bases - three within the GC pairs and two within the AT-pair. The term ‘soft’ refers to the well-known tunneling effect for H atoms in all hydrogen bonds, where the H atom is able to tunnel in any O-H...N hydrogen bond (please google for details). These findings need to be investigated further in particular as to how the environment-specific effects can be integrated within the program-controlled responses.

### 2.7. Coherence and growth by layers

The efficient energy reuse requires a spatially *consistent control* of growth, and that requires a *coherence - both spatial and temporal* - within a species. However, with an increasing differentiation, the decoherence effects begin to obstruct energy reuse due to differentiation-dependent spatial and temporal ‘inconsistencies’ in energy exchange and material supply. In addition, an advanced differentiation makes a species substrate (‘material’) less efficient and flexible as a conductor of signals and materials. In fact, due to advanced differentiation (in the grown species) only the internal ‘channels’ of a species still get involved in an active energy reuse/exchange due to the presence of active little-differentiated and easy-to-respond (micro)organisms such as viruses and bacteria. Combined, the differentiation and de-coherence make energy reuse finally drastically inhibited.

The growth by *layers* is another interesting implication of the energy reuse maximization rate. It is also a typical expression of history trait of a species. Why the growth of a species likely occurs by *layers or rings*? Within a multi-celled species, the available cells (generated by cell division) tend to get *organized* into spatial *layers* to be ‘deposited’ onto a species surface as a single integrated unit (vs. to attachments of separate cells). The number of growth rings(NGR) can be directly measured for plants and for many sea species. For example, extensive measurements of growth and longevity of bivalves [13] were very consistent in terms of the number of rings and longevity - up to 150 years. For animals including humans, the rings are not easy to detect and measure. Within a single cell the quasi-ring structures can be seen in cytoplasm [10]. At a tissue and organ level, some limited data on the ring-like structures are also available.

## 3. Exploratory approaches

The proposed mechanism opens a new dimension in research and developments but for now they are basically *exploratory* and need further discussions and input from experts in related fields. Here we are looking into few research options, the very first steps in an in-depth understanding of life dynamics and related applications. The standard ‘wet’ energy-driven molecular dynamics has the obvious performance limits. In addition, its guidance/control options are also very limited. So, any approaches that allow overcome these limitations are of significant interest.

### 3.1. Toward a high-speed competitive search.

In the *organic* world, the species competitive dynamics is *wet and protein-based*, and so quite *slow* in maximization of energy reuse and in building the protein responses in the growth process, a ‘side effect’ of the primary energy-reuse maximization dynamics. To explore the high-speed version of competitive search dynamics, the competition needs to be established in the dedicated ‘dry’ high-speed substrate. The promising candidates may be silicon, laser resonator, and similar substrates where the *high-speed* electronic degrees of freedom (DoFs), the modes, are available.

Silicon may be a promising option in implementation of high-speed competitive search. The process requires a non-stop generation of the variety of (electronic) states. Say, an external pulse can generate an excitation-like process which involves a set of chip-wide (electronic) charge-based patterns. If the spatial (and temporal) *constraints* get applied, the patterns *compete* to match the applied constraints which serves as a tester/filter. In the testing, the patterns get selected which *match* constraints. This is a high-speed non-stop sampling and testing similar the ones in the *wet* systems. Meanwhile, research and developments in the last decade indicate to a number of options to create the ‘learning’ silicon, silicon neurons [xx] thus opening a way to setup the charge-based memory patterns in silicon.

Such charge-based memory patterns may overlap in time due to charge accumulation (without erasing previous ones). This way a progress in sampling and testing can be seen as the overlapping (reinforced) memory patterns. When constraints get stable, the reinforced pattern gets stable too. This way, a one-way non-stop competitive electronic dynamics may be implemented on the chip, a kind of on-chip ‘living’ species with the high-speed control capabilities.

Then such a ‘hidden’ in-silicon competitive electronic dynamics can be made ‘visible’ by *coupling* an established memory pattern with an external process. One interesting option is to *couple* an electrical charge pattern of a mode in silicon chip to a (electrically) sensitive molecular process, say, protein or other synthesis, polymerization, growth, etc. This way, each charge-based memory pattern (a mode) in silicon becomes a spatial *driver* for a proper charge-sensitive application-specific synthetic molecular dynamics.

### 3.2. Modeling using Monte-Carlo methods

For in-depth understanding of the proposed mechanism, the modeling of the *competitive* sampling and testing phase is necessary. In particular, how the sampling dynamics ‘generates’ various species samples (configurations)  $S$ , including the ones in their excited states  $S^*$ , as well as the *matched* partners  $P$ . For modeling attachments  $S^* + P \rightarrow SP^*$ , the estimates for the proper rate constants need to be done or the rate constants need to be taken from the chemical reactivity databases. The testing phase focused on the  $SP^*$  lifetimes and their reactivities could be simulated using the estimates of the lifetimes and rate constants of the newly built  $SP^*$  pairs. The proper Monte-Carlo sampling methods will be explored with the modifications to include the reactivities (rate constants) of excited samples  $S^*$  and the  $SP^*$  pairs. In addition to the estimates, the available databases of the lifetimes will be used as well. Those research opportunities are planned to be investigated in the separate paper.

### 3.3. Proposed live experiments.

In-live experiments to demonstrate the major features of the proposed approach are of interest. The starting point is the *simplest* or *minimal* energy reuse system with search capabilities. The experiments by Gerald Joyce group at Scripps [7] and by George Church group at Harvard-MIT [8] are the very promising steps in that direction<sup>1</sup>. Silicon chip integration into a tissue/organ to facilitate a competitive energy reuse and - using an in-place feedback - to correct a specific biological function in-place is also an interesting and promising option.

### 3.4. Options to control the energy reuse rate

According to the proposed mechanism, the efficiency of energy reuse gets determined by the number of available degrees of freedom (DoFs), the energy spreading dynamics, and by the DoFs build-up rate. So, the DoFs increase by any possible methods is a *generic* approach to maximization of the energy reuse rate. Competitive sampling is a critical part of that dynamics, which generally occurs at molecular (actually, electronic) level. However, since long ago there has been understanding and the practical techniques of organism-level sampling enhancement - an additional option to generate extra DoFs and so enhance the energy reuse rate during human lifetime.

Although the internal competitive sampling occurs inside a species, it can also be enhanced by the *external* applying of ‘various gradients’. The possible ‘forces’ are mechanical, electrical, and others. The gradients in temperature, concentrations, etc applied in space and in time such as heat shock, concentration shock, radiation shock are the typical examples. The ‘shocks’ used to trigger a competitive energy reuse dynamics including protein synthesis in cells. For example, heat shock proteins (HSP) and other appropriate responses to the ‘unexpected’ shocks [11].

The external, organism-level enhancement of competitive sampling is an additional option available in the natural and/or man-engineered environments. This approach gets increasingly used in the recent decades to enhance sampling by generation *novel* DoFs using various man-engineered techniques. Some include the applications of ‘gradients’ - varying *intensity* of the actions/’forces’ applied to a species. These are the physical forces/loads, gradients of temperature, concentrations, etc. This also includes many man-engineered activities such as exercises with *varying* the number and intensity of possible movements and loads - to ‘activate’ various used to be ‘frozen’ (not used) human body DoFs. The *variety, intensity, and duration* are the key points here. The ‘uncommon’ movements - such as dancing, biking, swimming, walking, hiking, etc - anything which *expands* the human body/organism *configuration space* and/or make *flexible* the barriers between various segments of the configuration space. The relaxation, meditation, and similar techniques help to make it happen. This is basically only the beginning of the synthetic, human-engineered approach to the DoF sampling and testing which will include both molecular-level and species/organism-level sampling and testing techniques, a very promising area of enhancing energy reuse rate at both a human organism level and collective (social, super-organism) level.

#### 4. Conclusion: implications and further research

*A mechanism* of energy-driven non-stop *competitive* molecular dynamics proposed early [4] can be seen as molecular *search* aimed to find the molecular species with the best energy-reusing capabilities. It includes the growth and differentiation. The growth builds-up the DoFs needed for energy spreading. The *differentiation* by building membranes and compartments while minimizing energy loss at the same time increasingly obstructs energy reuse slowing it down until full stoppage. We link this universal phenomenon to *ageing* and finally to *death*. To slow down this dynamics, we propose the various options to enhance sampling dynamics and so to generate additional DoFs, in addition to the internal molecular mechanism

*Planet-wide implications.* In the process of non-stop planet-wide species growth aimed at maximization of the energy reuse rate, each winning species becomes an *optimal* energy accumulating engine. This process creates a ‘hidden’ non-stop planet-wide turnover/search dynamics aimed at building the best energy reusing species. The competition leaves only the best in terms of minimal energy dissipation rate. They are also the increasingly more complex and longer-living energy accumulators,

*Further research* is necessary to investigate the global implications of competitive energy reuse. Its applications in various conditions and environments - industrial, biomedical, healthcare, space, etc. are of significant interest. They include low-speed (‘wet’), high-speed (silicon, optical/laser and other), low/highly-intelligent, etc. applications. The man-controlled energy-reuse-based application-specific synthetic organisms - the next-generation ‘reactors’ - are the future-generation ‘things’. In such reactors, the ‘spontaneous’ growth of living matter gets enhanced and modified with control/guidance features which will allow for synthesis of ready-to-be-used (‘end-user’) application-specific organisms - living or ‘green’ things/objects. Options are available to use that search dynamics in other molecular applications such as synthesis of pre-specified products.

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