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Some Proposed Design Elements for Self-Organization Processes at Multiple Length Scales

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Abstract

We present an initial report on a new research effort to theoretically understand the self-organization processes at a variety of length scales in living systems. Our goal is to discover and develop design principles that will enable life-like self-organization processes to be created using non-biological components. A new set of theoretical concepts and design elements are presented and motivated by reference to certain biological self-organization processes. Two key features of this theoretical approach are: a statistical mechanics description of populations of active, far-from-equilibrium machines that carry out self-organization; the design of self-organizing machine components at large length scales through the active *mimicry* of thermodynamic properties at the nanoscale. The ideas presented here will provide the basis for a follow-on series of self-organization simulations that will explore the creation of self-organization in artificial (non-living) systems.

I. Introduction

One of the main goals of the current nanoscience initiative is to develop approaches for assembling nanoscale components into larger-scale, organized structures with desired properties and/or functionalities. Living systems accomplish this through a variety of self-assembly and self-organization processes. The technological appeal of achieving life-like self-assembly and self-organization in man-made materials and systems is clear. A recent BES Workshop on Complexity [1] has also made clear the timeliness of a concerted multidisciplinary research effort to understand and mimic these biological processes in artificial systems. A key research goal is the theoretical understanding of the *self-organized* design and assembly processes by which living organisms create materials and functional complexes at a variety of length scales.

In this paper we present an initial report on a new research effort to theoretically understand the self-organization processes at a variety of length scales in living systems. The theoretical ideas and design elements presented here will provide the basis for a series of self-organization simulations that will explore the creation of self-organization in artificial (non-living) systems. Our purpose is not to create a bibliography of the extensive literature on the current state of the art, and we refer the reader elsewhere for self-organization reference lists [3]. The paper is organized as follows. Section II outlines some of the specific scientific questions that motivate this research. The third section presents elements of the new theoretical approach we are developing for designing man-made self-organizing systems. Two key features of this approach are: a statistical mechanics description of populations of active, far-from-equilibrium machines that carry out self-organization; the design of self-organizing machine components at large length scales through the active *mimicry* of thermodynamic properties at the nanoscale. Section IV compares the expected properties of the proposed machine components against a few biological machine examples to support their plausibility. Section V discusses the relationship of these self-organizing systems to information processing systems. Section VI presents our conclusions.

II. Some Scientific Issues for Understanding Self-Organization

There are many scientific questions that must be resolved to understand and mimic self-organization at multiple length scales in biological systems. Important among these are the following issues.

IIa Relationships between self-organization processes at different length scales

Understanding how such self-assembly processes can occur at any one length scale is a key challenge. How are the self-assembling components constrained to carry out the appropriate actions at the right places and times? Further, the forces and transport properties relevant to self-assembly at one length scale are generally not the same as those for greatly differing length scales. For example, the thermal motion that dominates transport properties of nanoscale molecular structures plays little role in the transport of much larger structures. Thus, the physical details of a particular self-assembly process do not generalize to arbitrary length scales.

Living systems accomplish self-organization repeatedly across a vast range of length scales through *hierarchical* organization [1,2]. Successful biological systems have been able to utilize the available (self-assembled) biological components at any particular length scale, together with the available forces and transport mechanisms, to develop new and distinct self-organization processes at a larger length scale. This hierarchical organization is evident in the animal kingdom through the assembly of: proteins from amino acids; cells from proteins and other macromolecules; tissues and organs from cells; organisms from tissues and organs; social communities of organisms from individual organisms.

Despite the great differences in the self-organization processes at different length scales and hierarchy levels in living systems, there are intriguing patterns in self-organizing systems that recur at many length scales [4]. One of many examples is the strikingly similar stripe/dot patterns that occur in a variety of biological and non-biological self-organizing systems. Example stripe/dot systems include: nanosized structures in binary epilayers deposited on flat solid surfaces; Turing patterns in activation-inhibitor chemical reactions; and morphogenesis-based pigmentation patterns in animal pelts. The commonality in such patterns can be partly understood as due to similar underlying mathematics of the processes, even though the physical details that lead to the similar mathematics are quite different. It is presently unclear how or why self-organized processes of many different types and length scales should yield similar structural or functional patterns. Is this merely a coincidence or the manifestation of some undiscovered principle of self-organization?

IIb The role of collective/emergent behavior

One important contribution to the self-organization process is believed to be the collective behavior exhibited by the large populations of components that typically make up such systems. The collective behaviors in self-organizing systems go by many names. Two common terms are swarm/hive intelligence and emergent behavior. Emergent collective behavior is one of the fundamental (and perhaps least intuitive) concepts in complex system research. Collective behaviors are interesting for exhibiting complexities that are not present in the simple behaviors of the individual components themselves. These behaviors are usually only evident when there are sufficiently large numbers of interacting components, and arise through the many interactions of the components with each other and the environment. Some aspects of self-organization will evidently be emergent properties, while other properties may have to be designed in to the system components to achieve self-organization. Which properties belong in which category for self-organizing processes?

IIc Sustaining non-equilibrium states by self-organization

Another important aspect of self-organization in living systems is that it is associated with maintaining far-from-equilibrium conditions. This is in contrast to certain man-made self-assembly processes that rely on equilibrating processes to generate order. Equilibration-based ordering is typically associated with non-functional components for which sources of energy are supplied only during assembly. Living systems as a whole persist in non-equilibrium states by continually harnessing an external source of excitation. The far-from-equilibrium configurations of living systems balance this excitation against the continual relaxation towards equilibrium. There are equilibration times associated with the system components that are in effect lifetimes for them. All of the components eventually lose their internal organization (and fail). The component population of such self-organized systems must be dynamic, in that old or failing components must be removed from the system, while newly built or acquired components take their places. There are mechanisms for the detection of aged, broken or improperly functioning components. This renewal process is a part of the continual flow of material in and out of the non-equilibrium living system. The component population as a whole can persist for time scales far longer than the characteristic lifetime of the individual components. How do all of the above characteristics arise in living systems? How can non-equilibrium states interact with each other and with an external source of excitation to maximize the persistence of far-from-equilibrium conditions?

IId Agent vs. physics theoretical descriptions

Complex phenomena at the nanoscale are naturally modeled using physics and chemistry to describe the interactions and thermal fluctuations of the molecular building blocks. Complex phenomena at the macroscale are often modeled using autonomous agents that execute simple algorithms and communicate with their peers and the environment. The use of very different theoretical descriptions for self-organization processes at vastly different length scales is not surprising given the discussion in Sec. IIa. However, if there are fundamental underlying principles of self-organization that extend across many length scales, then a more unified theoretical description may be possible. Can elements of these different theoretical approaches be merged to understand systems that span the entire range of length scales from nanoscale to macroscale?

IIe Measuring complexity and self-organization

There have been many proposals for defining and quantifying complexity, but there is no universally accepted one. How does one objectively measure the extent of self-organization and hierarchical structuring in a model system to evaluate model performance? The measure must directly depend on the amount of order achieved and should also reflect the size or number of components that have been organized.

III. Proposed design elements for self-organizing processes

The design elements that we propose for self-organization processes are well illustrated by the process of bacterial chemotaxis. This process is described first, followed by an outline of the key design elements.

IIIa Chemotaxis considered as a self-organization process

In comparison to the rapid thermal motion that drives much of the molecular activity at the nanoscale, the thermal motions of large bacteria are relatively slow. Some bacteria can act as machines that propel themselves with flagella. Chemotaxis is the process where such propulsion is generally towards increasing concentrations of attractive stimuli and generally away from others. Interestingly, these bacteria do not "swim" directly towards a food source, but execute a sort of random walk that resembles the diffusive motion of molecules at the nanoscale. This motion consists of alternating periods of tumbling (that randomizes the swimming direction) and straight swimming. The bacteria only need to bias the straight swim times (longer/shorter if larger/smaller amounts of food are detected this path compared to the previous straight path, respectively) to statistically converge to the highest concentration of food. An ensemble of bacteria, randomly placed in a region that contains a localized food source, will concentrate in the small region of greatest food supply after executing many cycles of stochastic tumbling and straight swimming. These bacteria are organizing their locations to a smaller, preferred volume, i.e. they are acting to reduce the spatial component of their entropy. Alternate forms of the chemotaxis process are important capabilities for many single-celled and multicellular organisms.

IIIb. Statistical mechanics description of self-organization processes

The chemotaxis example illustrates the important role that active ordering, i.e. entropy reduction, plays in our approach. A complete theoretical description of many other complex self-organization processes must handle large populations of active, interacting machines. We are developing a statistical mechanics picture to describe the non-equilibrium populations of active machinery that carry out self-organization processes. The natural metric for active ordering (i.e. self-organization) in such a picture is the system entropy. We will in fact base our measure of self-organized complexity, Cso, on entropy as follows:

$$\text{Cso} = S(\text{corresponding equilibrium state}) - S(\text{current state}), \qquad \text{(Eq. 1)}$$

where S is the usual statistical entropy (given by $S = k*\log W$, where W is the phase space volume accessible to the current state and k is the Boltzmann constant), and the entropic difference is between that of the actual non-equilibrium macrostate of the system and the corresponding equilibrium condition that it would relax to. This measure captures the dependence of complexity on order (the measure increases as the entropy of the current state decreases) and on size of the system (the upper limit on this measure is determined by the corresponding equilibrium entropy, which generally increases with more components in the system). As is well known, the statistical entropy remains a valid concept in non-equilibrium systems. The entropy of a collection of machines can be reduced by: reducing the phase space volume (including the physical volume) accessible to individuals; coupling the machines so that they do not act independently, thus reducing the degrees of freedom and the available phase space of collections of machines.

In hierarchical systems, the phase space volume W simplifies into separate factors for each hierarchy level. For example, consider a "cell" boundary that encloses n internal components. The degrees of freedom of the [cell + contents] can be factored into "external" ones (e.g. the external volume available) and "internal" ones (for various internal arrangements of the n components). This factorization can repeatedly continue for internal structure of each of the n components down to the molecular level. This allows the complexity measure to be a sum of entropy reduction contributions from the separate hierarchy levels. The extent to which system ordering is hierarchical can be quantitatively related to the extent that this entropy factorization occurs.

IIIc Nanoscale thermodynamic mimicry

The stochastic motion of bacterial chemotaxis motivates another key aspect of our approach. We hypothesize that successful self-organization machine behavior across many length scales can be achieved by generating behaviors (e.g. stochastic propulsion) that mimic the thermodynamic properties (e.g. rapid thermal molecular motion) of self-organizing biological machines at the nanoscale. These behaviors generally must be generated by the machinery at the larger length scales because the relevant physical forces and material properties do not resemble those of the nanoscale. The idea here is that the successful properties of nanoscale self-organization can be effectively reproduced to achieve self-organization at larger scales by active mimicking of these properties (by using different physical mechanisms). This design approach, if successful for artificial systems, will generate self-organizing processes at large length scales that are simultaneously different in physical detail from the nanoscale structures yet exhibit similar patterns of corresponding functionality. It would thus provide a resolution of the scientific issue in IIa above.

The unique combinations of properties exhibited by proteins and organic macromolecules are the mimicry targets of interest. These properties include thermal motion, attractive and repulsive molecular interactions, weak and strong (covalent) bonding, molecular recognition sites, allostery (physical shape changing) and the ability to carry out physical work. From this theoretical point of view, a bacterium might be considered to be effectively mimicking the randomness of diffusive thermal molecular motion at the micron size scale when it generates its own tumbling motion. The net motion of a bacterium towards a useful chemical source during chemotaxis might be considered as mimicry of a weak attractive force.

Further, this theoretical viewpoint suggests one particular pathway to the successful evolution of complex multicellular organisms and colonies. Organisms may self-organize in new ways at larger length scales if they "discover" how to harness available physics and material properties to mimic the properties of living systems at the nanoscale (i.e. the properties of proteins and organic macromolecules). This concept can be explored through the use of computer simulations.

IIId Carnot cycle generalization -- entropy pumps

Thermal entropy can be reduced in a local region through the use of cyclical heat engines (refrigerators) that "pump" heat and the associated thermal entropy out of a local region and dump it into the external environment. Heat pumps produce order at the molecular nanoscale. However, the hierarchical structure of large-scale self-organized systems means that much of the system entropy will be in *non-thermal* degrees of freedom. For example, the concentrating of bacteria to a small volume in the chemotaxis example above reduces an entropy component at the organism hierarchy level that is distinct from the entropy contribution of molecular motion. Heat engines will not be effective in extracting non-thermal entropy contributions associated with large scale structures.

The nanoscale mimicry principle described above leads us to propose novel machines that mimic/generalize the functioning of heat (entropy) extraction by conventional refrigerating heat engines, but which act on larger scale contributions to the system order. We will call this new class of entropy extracting machines entropy pumps, and note that their actions are essentially generalizing or mimicking the Carnot cycle. These machines will directly order the system around them by "pumping" or extracting non-thermal entropy out of each level of the hierarchical systems. We expect that specific pumps will be needed for each of the macrovariables at each hierarchy level. Some general properties that we expect for these machines are:

Entropy cycling – The machines must cycle one of their own macrovariables between low and high entropy values in imitation of the thermal entropy cycling of the working fluid in a heat engine. One way that machines can achieve this is by varying the macrovariable in a stochastic fashion (for high entropy states) or a deterministic fashion (for reduced entropy). For example, the bacteria exhibiting chemotaxis alternate between stochastic motion and straight motion.

Selectivity mechanism – The machines must have a method for recognizing other materials or machines with the relevant macrovariable and estimating whether the associated entropy is relatively low or high. Refrigerating heat engines achieve this automatically through the temperatures of the cooled region and the external environment. *Only heat* (and not material or some other undesired property) is selectively transferred to and from the working fluid as it interacts with the cooled region and the external environment. The machines we propose must supply this selectivity to mimic the entropic pumping action of heat engines. The corresponding property of bacteria in the chemotaxis example is the sensing of improving or degrading food content during motion.

Affecting variables during one half cycle – The entropy pump must preferentially act during the entropy decreasing part of the cycle in order to generate a net entropy decrease. This corresponds to the working fluid in a heat engine taking on and transporting heat during half of the Carnot cycle. The heat must not be brought back during the other half of the cycle, and is dumped to the environment to avoid this.

These entropy pumps must all be powered to do their work, and this power must ultimately result from a continual source of external excitation. The lowered entropy that results from the initial capture of the external excitation is lost as it is used to drive an entropy pump. This process allows the entropy pump to reduce the entropy associated with another system variable. Thus, the entropy pumps may be viewed as simply transferring a portion of the lowered entropy from the initial excitation to another part of the system.

IIIe Selective constraints to maintain reduced entropy

An entropy pump reduces the phase space volume associated with a set of components, but these components will not generally remain in a low entropy state after pumping unless constraints are introduced that continue to constrain the allowable phase space volume to this reduced value. Another class of machine components is needed to provide physical constraints that can be selectively introduced to maintain the low entropy conditions that are generated by the entropy pumps. A simple example of such a component is a closed physical membrane that acts as a spatial container. Non-equilibrium concentrations of useful materials can be established within such membranes by pumping material through gates/openings, effectively "storing" the lowered entropy generated by the pumping action.

IV. Comparisons to living machinery

We propose that key design elements of artificial self-organizing systems are populations of entropy pumps and selective constraints to preserve entropy reductions. We further hypothesize that related machines should be ubiquitous in living systems at every length scale. Of course, not all cyclic processes in Nature involve entropy cycling. An open question is the extent to which various cyclic activities in biosystems may be consistent with these non-thermal ordering mechanisms.

Here we briefly list a few examples of biological systems and activities at different length scales that are evidently consistent with this picture. Many activities of social insect colonies appear to fit this viewpoint. For example, foraging behaviors include cycles of stochastic searches and deterministic following of trails to discovered food sources. Foraging ultimately reduces the spatial entropy associated with initially dispersed food sources by concentrating the discovered food in the colony nest. Social insect colonies also carry out a variety of entropy-reducing sorting, stacking, aligning, and building activities. Certain processes that occur in the membranes of eucaryotic cells also fit this picture. For example, ion channels and ion pumps create a cycle of reducing the entropy by creating a gradient of a chemical component and then increasing the entropy by allowing ions to approach equilibrium by unimpeded flow back through the membrane. The material of the cell membrane itself and the bound membrane receptor proteins are cycled by the continual ingesting of small portions of membrane into the inside of the cell (pinocytosis) and the continual restoration of membrane material by the merging of internal organelles with the membrane. Pinocytosis is the entropy-increasing part of the cycle, as more degrees of freedom (more organelles) are created in the process. The overall cycle acts as an entropy pump to bring external proteins that have been captured by the membrane receptors into the interior of the cell membrane (with a greatly reduced accessible volume compared to that external to the cell). Machines that generate their own motion according to alternating cycles of high-entropy stochastic motion and low-entropy deterministic motion can trace out complex branching patterns that can be useful for assembling complex structures. We are envisioning structures such as ant colony nests with alternating tunnels and large chambers, branching tree structures and vascular networks.

We also list a few examples of selective constraints that store or preserve the entropy reductions created by the entropy pumps. Physical containers fit into this category. Thus, cell membranes, organelle membranes, organism skins and insect colony nests all serve to preserve spatial entropy reductions at different length scales. Temporary binding of materials also serves to retain spatial entropy reductions. Another type of constraint includes structures that limit the direction of transport of moving material or mobile machines. The non-branching segments of chemical trails and nest tunnels created by social insects, microtubules in eucaryote cells and game trails all constrain the directions of transport to essentially one forward and one backward option. In contrast, branching structures can impose entropy increases or decreases (depending on the direction of flow) on materials and machines constrained by them. For example, blood cells pumped out by the heart into the arteries experience an increase in volumetric entropy as they take alternate paths through the increasingly branched network. The blood cells that return through to the heart complete an entropy cycle by converging from many locations to one (the heart).

V. Connection to information processing systems

A property of interest for entropy-reducing systems is their information processing capabilities. One of the interesting developments in statistical mechanics was the gradual realization of the deep connection between information, computation and statistical mechanics. Shannon's measure of information has the same form as Boltzmann's statistical entropy, and it is now understood that this is not merely coincidental. The information content that one has about a physical system is measured by the ordering of that system, i.e. the negative of the entropy. The 2nd law of thermodynamics would be violated by certain information processing devices (the so-called "intelligent" Maxwell's demons) unless information is regarded as truly physical. There are true thermodynamic (entropic) costs to the disposal/erasure of information in a computing machine [5].

The flip side of this information-entropy relationship is that physical systems that self-order must be regarded as machines that generate and process information. Self-organizing systems should in fact act as information processing systems in general. It is perhaps easy to see that structural ordering provides means for storing information. In addition, our preliminary work suggests that the cyclic entropy pumps can act in an algorithmic way. Algorithms for sorting and biased-diffusion naturally arise from the actions of different versions of entropy pumps. An interesting direction for future work is the exploration of the variety of algorithmic behaviors that can result from our self-organization design approach. This also provides a connection between the theoretical physics and algorithmic models applied at vastly different length scales for the same hierarchical self-organizing systems. This may provide the basis for a consistent theoretical picture of self-organization across all length scales.

VI. Conclusions

We have presented and motivated a new set of theoretical concepts and design elements from our new research effort aimed at understanding and mimicking biological self-organization processes at a variety of length scales. Two key features of this theoretical approach are: a statistical mechanics description of populations of active, far-from-equilibrium machines that carry out self-organization; the design of self-organizing machine components at large length scales through the active *mimicry* of thermodynamic properties at the nanoscale. The next stage of this work will involve further development of the model and computer simulations of the self-ordering properties and collective behaviors that result from populations of the machine components described above.

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