Emergent natural surfaces and the evolution of novel biological surfaces

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Main idea/Introduction

**Goal:** to stake out territory for “unified theory of self-assembly”.

**H:** emergent phenomena, evolution by natural selection and neutral processes, and biological development are all part of same subject, self-assembly of biomaterials.

**Wikipedia:**
"disordered system of pre-existing components forms an organized structure or pattern as a consequence of specific, local interactions among the components themselves, without external direction".

1) **Self-assembly vs. 2) Self-organization:**
1) ordered state forms as a system approaches equilibrium, reducing its free energy, 2) patterns of pre-existing components organized by specific local interactions.

**WhatIs.com:**
"objects, devices, and systems form structures without external prodding".

**Biology-Online.org:**
“property of forming structures from sub-units without any external source of information about the structure to be formed”.
Introduction/Basic predictions

Prediction #1: surfaces will be shaped by an intimate relationship with its function (neuromechanical approach of Full and Koditschek, J. Exp. Bio, 1999).

Prediction #2: there are “assembly rules” for materials that are recapitulated in development according to their overall stability.

* one example: morphogenesis (Turing’s model of algorithmic pattern formation).

Prediction #3: multilevel environmental selection may act at any level of organization, from the entire surface to the molecular scale.

* environmental pressures act upon biological processes to form compliant (rigid but flexible) surfaces at various scales (from accretions to sheets of material, composites).
Prediction #1

All novel, highly-specialized surfaces

* in example at right, hydrophobic leaf tissue at three scales.

* functionally and structurally embedded in larger-scale structures.

* example: components of microscale arranged in parallel to form mesoscale.

* example: need for function at mesoscale determines form at macroscale.

* must be parameterized using kinetic, surface, and other models.

* parameterization: range of values under which system will perform in particular configuration.
Prediction #1 (con’t)

Material and structure that constitute the surface of the gecko footpad (Shah and Sitti, IEEE Intl. Conf. Robotics and Biomimetics, 2004):

* specialized for grasping, walking, running on vertical surface.

* hairs at microscale interact via Van der Waals forces, produces “stickiness” at mesoscale, agility at macroscale.

Co-evolved with both local biomechanical function and organismal movement behavior.
Prediction #2

As surfaces are assembled in a developmental phase, those of high functional fitness must be stable in function, formation.

* only a subset of all possible system configurations are workable in a functional context.

* functional fitness relative to other like structures at same scale.

* functional fitness is a measure of surface stability during function, interaction with other surfaces.

* for *in vitro* materials, fitness is based on range of parameters relative to introduced stresses.

* evidence for this comes from developmental gene expression and tissue formation, which is highly regulated in time, space, and scale.
Prediction #2 (con’t)

The initiation of tissue maintenance mechanisms:

Unfold in a similar way
(Reeves et.al, Developmental Cell, 2006)

* stresses and other stimuli trigger developmental, inflammatory, and growth pathways.

* provide a more stable and adaptable surface over the life-course of the material.

* contribute to functional fitness of material.

* tissue maintenance responds more quickly or to a wide range of parameters = increase in functional fitness.
Attributes of Model: selection and synchrony

The concept of synchronicity is helpful for understanding how selection acts at these different scales.


* sync = temporal organization of related physical objects (oscillators, processes).

* relies on a physical form of communication (e.g. firefly luminescence, resonant motion)
Attributes of Model: selection and synchrony (con’t)

Selective pressure that is in-phase and ubiquitous at every level of the system:

* predicted to have a transformative effect on the surface.

* coordinated selection on all scales at the same time can cause large-scale changes to system (phase transition).

* allowing for novel surfaces to aggregate.

* environmental selection provides directionality to emergent processes.

Strong environmental selection = strong emergence, while weak or no (neutral) selection = weak emergence.

Example:
Phase transition at macroscale occurring at one part of surface.
Attributes of Model: selection function and replicators

Selection function explicitly derived:

* by treating each component of the surface as a replicator.

* replicator = object that is capable of self-renewal or (cells, self-assembling structures).

* networked automata approach (see at right).

* replicators either compete or cooperate with other replicators (evolutionary dynamics, (Nowak and Ohtsuki, PNAS USA, 2008).
Attributes of Model: cooperation


In the case of cooperation, emergence may also act in a neutral manner:

Lack of direct selection:

* in this case, replicators cooperate and produces anisotropic composite materials.

* when selection for single type of element or structure predominates, materials are more homogeneous.

* production of stable polymers, ultra-specialized tissues, and novel phenotypic structures.
Emergent phenomena and evolutionary processes (dynamics):

1) Work in tandem

* in a manner analogous to biological and non-biological surfaces (e.g. feet running on sand, rock).


Play a critical role in:

2) Initial formation

* setting up initial condition for system – selection then emergence.

Sustained maintenance of materials and structures in vivo.
Model of Evolutionary Dynamics and Emergence (con’t)

Different configurations of molecules, polymer morphologies, and surfaces have specific functional fitness.

* molecular species, polymer types, and surface types can form populations.

* functional fitness determines each unit’s role in strong or weak emergence.

Natural selection:

* high fitness polymers – responsible for strong emergence.

* low fitness polymers – responsible for weak emergence.

* high fitness – building blocks, exhibit synchronized behavior.
Model of Evolutionary Dynamics and Emergence (con’t)

Selection (sorting by functional fitness) acts at three scales:

* individual molecules (e.g. hydrophobic, hydrophilic).
* polymers (e.g. binding affinities).
* surfaces (e.g. water-air interface, lipid bilayers).

Neutral processes: occurs as a consequence of population restriction (in size).

Small changes (at smallest scales) have no consequences on functional fitness (larger scales).

* acts to shape molecular, polymer population, surface characteristics without selection.
* surface made up of polymers of a similar geometry (homogeneous).
* selection, drift act up a population of polymers, set up stable, unstable regimes.
Example of relationship of self-assembly to:

- selection (forces from environment)
- neutrality (Young’s Modulus)

At a single organizational scale.
Model of Evolutionary Dynamics and Emergence (con’t)

Replicator: elements with highest functional fitness form functional units.

* these units form patterns that are highly repeatable (fractal).

* examples: tree bark, lizard skin.

* in many cases, internal (gene expression) and external (air, water pressure) serve to impose conditions for replication.

Take home message (key attributes of self-assembly potential):

1) self-assembly process can initiate, amplify, dampen selective and neutral processes, determine statics and dynamics of surface.

* process: acquiring functional fitness, selection, aggregation, function (recursive).

2) functional fitness and ability to replicate as cooperative unit.
Selection at a single scale

Selective pressures that are limited to a single scale:

* have a limited effect on pushing system towards a novel state.

* has a deleterious effect on stability.

Selection can be imposed by natural forces, or applied artificially to construct nanoscale devices, tools.

DNA Brownian Walker, Omabegho et.al, Science, 324, 67-71, 2009
Synchronized Surface Example

Lattice of inflatable membranes (excitable, electroactive structures):

Coupled Fitzhugh-Nagumo equations:
Paired membranes depolarize/recover in unison or with degree of lag.

\[ V_n = V_m - \frac{V_m^3}{3} - W_m + I \]
\[ W_m = 0.08 (V_n + 0.07 - 0.08 W_n) \]

\( V \) = membrane potential, \( W \) = recovery variable, \( I \) = magnitude of stimulus current. \( m \) and \( n \) = neighboring membranes.

Selection, neutral processes imposed upon population of membranes:

Prediction: evolutionary dynamics impose stable regimes (synchronized patterns of coupled activation, regional changes in surface tension).

Izhikevich and Fitzhugh. Scholarpedia, 1(9), 1349.
Self-assembled Surface Example

NKS (computational) approach:

* rules applied to an emergent system produces complex behavior and properties.

Intrinsic generation of randomness:

* given an initial condition, system forms patterns according to simple rules.

* in such systems, very complex patterns emerge

* patterns are highly repeatable (contrast with randomness = environmental perturbation).
Future applications:

* biomechanical studies
* nanotechnology/nanorobotics
* understanding the "phenome" for highly-specialized traits of interest (Freimer and Sabatti, Nature Genetics, 2003).
* design process of innovative biomimetic applications.

How complex biological structures (gecko’s foot) can be built artificially.

How multiple surfaces were formed and interact with larger biological structures.

How complex surfaces and phenotypic structures are derived from genes and proteins.