#### The BIG Picture...

By trying to build a coral reef, we stand a good chance of identifying Natural Laws that can be applied to ALL ecosystems (natural & man-made).

#### Biogeochemistry is complex & hard to control...

Tens-of-millions of life forms, mostly phage, call coral reefs home. All of these diverse life forms are interacting with each other in ever changing ways & all of this activity occurs within the dynamical Gaian biosphere. This makes coral reefs incredibly complex. And it is difficult to control complex things:

we are going to need some mathy help, &
we also need a common lexicon

#### Main Mathy Ways to Describe Complex Systems

## Analytical Models $\frac{dx}{dt} = \alpha x - \beta xy$ $\frac{dy}{dt} = \delta xy - \gamma y$

PDEs: linked sets of partial differential equations

Systems Dynamics & Complex System: non-linearity & emergent properties Network Theory: identify interconnectivity & interdependencies

#### Statistical Models $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k + \epsilon$

Multivariate: many statistical variables at the same time

Machine Learning: identify patterns & behaviors from large datasets

#### Mixed Models & Simulations $U_i(s_1^*, ..., s_i^*, ..., s_n^*) \ge U_i(s_1^*, ..., s_n^*)$

Stochastic: statistical inputs into analytical models Agents & Game Theory: decision-making entities

#### Main ways to "control" complex systems

#### **Control Theory**

Uses analytical & mixed models. The main control techniques are feedback control (e.g., PID controllers), feedforward control, and robust control.

#### Statistical Process Control

Uses statistical models. Monitor a process through the use of control charts to detect and control for variability in the process. Feedback loops are implicitly present in SPC.



#### Feedback Loop Analysis

Analyzing and designing appropriate feedback loops is essential for maintaining control over a system.

#### Central Feedbacks Related to Coral Reef Arks

#### DOC-Disease-Algae-Microbes (DDAM)



Wholobionts



Which feedbacks are important for building a coral reef?

These will be positive, biogeochemistry feedbacks that will include: 1) viruses, & 2) the Hermit Crab Loop :)



P.H.A.G.E.S. & the Goldilocks Rule are a qualitative-toquantitative framework for understanding ecosystems.

#### A main goal is to predict what happens at a future time point for a biological system like the Arks



## Things are multidimensional



A steak is multidimensional, ranging from its physical x, y, z position in space to measures of the steak's nutritional value (e.g., Calories, vitamins, protein, fat...).

Note that all dimensions (e.g., micronutrients) can be expressed in lower dimensional terms, all the way down to the base metric units. Even if we need new base units.

## Cross-sections of the time vs things on a graph are *static* snapshots



Arrows are P.H.A.G.E.S. processes

## ? Is a steak good for you ?



A steak's nutritional value is dependent on person's History. To someone starving, a steak is extremely nutritious. To an obese person, a steak is another step towards a heart attack...

The Goldilocks Line helps determine "goodness"

## The Goldilocks Line

At any point in time, every living system either has an excess of either electron-donors (e.g., sugar = solid) or electron-acceptors (e.g., oxygen = gas).

The Goldilocks Line divides the biosphere into electron-donor rich or electron-acceptor rich static snapshots.



In general, Macrobes like the electron-acceptor side of the Goldilocks Line, whereas the Microbes like the electron-donor side.

Think of fresh air versus an anoxic pond...

## ATP, work, & oxygen



high-energy electrons from the steak flow through central metabolism to lower- energy orbitals in the electron-acceptors

If there are excess electron-acceptors (e.g., oxygen), then the steak is converted to ATP, CO<sub>2</sub>, & H<sub>2</sub>O.

# The process of converting food into ATP is called catabolism



ATP is necessary to do work, like running, lifting, thinking, & build a coral reef

## Catabolism predominates when electron-acceptors are in excess.

Viralized



## Sugar & biomass



the digestive system breaks the electron-donor steak into small molecules that can be absorbed into central metabolism

If there are excess electron-donors (e.g., sugar), then the steak is mostly converted into protein, fat, & DNA to build more biomass

# The process of building more biomass is called anabolism



too many electrondonors from food & you will get fat OR build muscle if you combine it with exercise



Anabolism predominates when electron-acceptors are limiting. Microbialized

#### As you might expect, healthy organisms & ecosystems need a mixture of anabolism & catabolism



Therefore, the "goodness" of the steak is dependent on your goals & history.

What should be our goals for the Coral Reef Arks? Line Islands as the Baselines

State Variable	Rationale	Measurement	Set Point
Virus-to-Microbe ratio (VMRs)	reverse microbialization	epifluorescent microscopy	>12
Calcification	shoreline protection	buoyant weight	>500 g m² year
Aesthetic	tourism	photos (Haas et al. 2015)	<20 Aesthetic Score
Fish	food	visual surveys	>50 g m <sup>2</sup>
Biodiversity	conservation	sequencing	>4.5 Shannon Wiene
Chemical diversity	drugs	LC-MS/MS	>5.5 Shannon Wiene

#### Control Theory is an approach to predictively manipulate dynamical systems

build dynamical models of the Arks measure state variables decide on set points (i.e., values of state variable) How close are the state variable values to set points? manipulate control process variables to move toward set points



## **Control Process Variables**

#### Location

- increase oxygen fluxes by targeting high flow sites

### Geometry

- habitat for animals, particularly zooplankton

#### Materials

- enhance recruitment of calcifiers

#### Biomanipulation

- stocking with precolonized ARMS vs passive
- enhance algal grazing

### All we need is a good model...

## The BioToy Universe

#### Goals

I. Establish a physical toy model for studying living Systems

- > sufficiently simple to make the model mathematically tractable
- > sufficiently complex to provide insight into coral reefs & Arks
- > utilizes lessons from Finite-Time Thermodynamics (FTT)
- II. Establish terms & symbology for discussion & math
  - > to facilitate discussion we need agreed upon terms
  - > easier for new members to the discussion (e.g., incoming students)

Thermodynamics & Statistical Thermodynamics are still the best known approaches for understanding problems ranging from fundamental to practical.

## Starting Point for Terms & Background

Autopoiesis	A system's property of being able to maintain and reproduce itself
Compensated heat (Qc)	The exergy dissipated as heat which is necessary to satisfy constraints
Constraint	A conditional requirement of the feasible set of solutions to an optimization problem
Degree of freedom	An independent coordinate, describing the state of a system, along which change can occur
Dissipation	The degradation of energy available to do work
Dissipative structure	An open non-equilibrium thermodynamic system that generates order spontaneously by directing
	streams of exergy
Emergy	The amount of exergy that is either directly or indirectly required to drive a process
Entropy (S)	Entropy is a thermodynamic state function whose change is equal to the heat received by the
	system divided by its temperature. See also Box 1.
Exergy	The work that could be extracted in a process that reversibly brings the system to equilibrium with
	the environment. See also Box 1.
Far-from-equilibrium system	Systems subjected to flows of matter and/or energy, in the non-linear regime
Fitness	The ability of an entity to survive and reproduce. Fitness is the quantitative parametrization of
	selection in evolutionary biology
Functional control region	The region between minimum dissipation operation and maximum power operation
Heterotroph	An organism that cannot fix carbon from an inorganic source, so it must consume complex organic
	molecules that have been previously anabolized by another organism
Informed	Structured by the passage of information from a previous time
Near-equilibrium systems	Systems in which flows are linear in the forces
Ontogeny	The development of an organism from the time of its inception (e.g., fertilization) to its mature form
Orientor	A variable that describes where a system tends move in state space
Pareto optimum	A set of states which optimizes a combination of two or more objectives (e.g., maximum power and
	minimum dissipation) where an improvement in one objective cannot occur without the worsening
	of another
Power	The rate at which work is done
Selection	The differential reproduction and survival of a particular type. Selection is the key mechanism
	behind evolutionary change
Spontaneity	The maximum work obtainable from a reversible flow of an extensity
Succession	The process of sequential change in the structure of an ecological community as the ecosystem
	matures
Unit of selection	Any entity in the hierarchy of biological organization that is subject to natural selection and
	subsequent change over time
Waste heat (Q <sub>W</sub> )	The heat dissipated above and beyond the minimum necessary to achieve the specified rate of the
	process subject to constraints

#### Roach et al. (2018) JNET

## The BioToy Universe



> the living System is a Black Box

> the Surroundings include water & the Sun plus the Earth's mantle, which supply the ionizing radiation splits water into  $H^+$  &  $O^-$ 

> remember that Energy is transferred ONLY as Work or Heat

The Boundary between the Surroundings & the System can be changed for thought experiments

#### All life preys upon $H^+$ & O<sup>-</sup> to form $H_2O$ & do Work

> formation of one mole of water from hydrogen & oxygen is exothermic and releases ~286 kJ Energy. THIS IS THE ONLY ENERGY SOURCE!

- > the energy is used to do Work
- > Work (W) = pV; where p is pressure & V is Volume



The H<sup>+</sup> & O<sup>-</sup> are supplied by ionizing radiation from the fusion from the Sun or fission from the mantle

## Thought Experiment 1: The Ty-Is-Still-Not-Working State



the boundary is:

flexible or inflexible

- volume can change or not

diathermic or adiabatic – transfers Heat or not

semi-permeable to: nothing

#### After infinite amounts of time ( $\tau$ ) passes no Work has been done...

## Thought Experiment #2: The Segall-Working-All-the-Time State





the boundary is:

#### flexible

- volume can change

#### adiabatic

- no Heat transferred

semi-permeable to: H<sup>+</sup> & O<sup>-2</sup>

The Volume of the system continually increases as a function of time as water is formed inside System

### Thought Experiment #3: Catalysis versus No Catalysis



If we open up the Systems & look, then we observe a piece of platinum metal inside Ark1 that is catalyzing the formation of water.

#### Thought Experiment #4: The State Function Volume is Path Independent



The amount Energy released by formation of water is fixed.

All Energy from water formation is converted to Work and observable as a change in the Volume.

We cannot tell if Ark1 & Ark3 are the same from the outside because there is an equal Volume change.

As the H<sup>+</sup> & O<sup>-</sup> move along the path back to water, there are two main points to consider: 1) are Thermodynamic Length (L) of the path, & 2) # of Steps (k) along the path

## Chemistry & Steps

> most biological Problems are directly related to chemical bonds

> formation & breaking of each chemical bond is a series of Steps (k) along a path of a specific Thermodynamic Length (L)



### Thermodynamic Length (L) & Steps (k)



Ladder Theorem expressed in Work

 $W_{lost} \ge \frac{L^2}{2k}$ 

Thermodynamic Length (L) is the distance between equilibrium states plotted on a Riemannian manifold.

In living systems, each step is catalyzed by an enzyme.

Salamon, Nulton, Ihrig (1984) J Chem Phys Salamon, et al. (2023) Entropy

## The enzymatic catalysts between all of the intermediates in metabolism are Steps (k)



> the total
Energy is still
constrained by
the number of
waters formed

Hypothesis: The genetic material records ALL of the Steps & the Steps are species specific.

#### Work is maximized by adding an infinite number of infinitesimal, reversible Steps (k)



Ladder Theorem expressed in Work (instead of Entropy)

$$W_{lost} \geq \frac{L^2}{2k}$$

This figure represents a special case where either the two systems are identical inside or the differences of L & k are equal.

The Ladder Theorem is built on geometric axioms (i.e., true). Applying it to biology may lead to a new Natural Law.

## The Tropical, Underwater BioToy Universe

Solar irradiance is relatively constant & direct at the equator. Therefore, we only need to consider ionizing energy captured in the largest area through the Ark.

Useful ionizing radiation is restricted to PAR, which is attenuated with depth.

PAR at 10 Meters Depth ~70 watts per square meter

This can be our initial constraint on exergy...



#### Surface Area & Volume

We assumed that a smaller Surface Area to Volume ratios would be good because all the creatures living in the Ark would be grazing the surface (e.g., fish).

In actuality, we mostly recruited planktivores & piscivores.



We may have been thinking about this wrong. The USEFUL volume (e.g., habitat) is decreasing & we aren't getting enough predation on the surface competitors of corals.

#### **Fractal Spheres**

- maximize internal volume/habitat for different sized organisms -

Need to keep hole sizes large enough that biofouling doesn't lead to microbialization of internal volumes.

Jenna Aquino's data suggests that the holes should be >4 cm...based on VMRs:)

Volume changes within this additional space (e.g., biomass including calcium carbonate) is the Work supported by the exergy.



Hypothesis: Work > Exergy<sub>ionization</sub> will reverse microbialization.

#### What I hope I said...

1) By trying to build a coral reef, we stand a good chance of identifying Natural Laws that can be applied to ALL ecosystems.

2) We need math models, a common language, and complimentary experimental systems (e.g., Arks). P.H.A.G.E.S. plus the Goldilocks Line is a good starting place.

3) A pro-calcifier Point-of-View is a reasonable goal to guiding our endeavors (i.e., try for the baselines derived from the Line Islands).

4) It is essential to identify positive feedback loops that will reverse microbialization.

5) To hunt deeper theories &/or laws, the Ladder Theorem is a good starting place. I am specifically proposing a thermodynamics framework call BioToy for thought & physical experiments.

6) Hypothesis: Work > Exergy<sub>ionization</sub> will reverse microbialization.

#### Coral Reef Arks

<coralarks.org>

#### data, various Arks projects, contacts, publications

Coral Reef Arks Home about projects people publications meetings donate

Coral reefs are some of the world's most beautiful and valuable ecosystems.

#### P.H.A.G.E.S. <coralandphage.org>

#### terminology & approach SDSU BioMath (1 pm PT on Fridays...email FLR)

#### P.H.A.G.E.S.

P.H.A.G.E.S. was originally proposed as a popular science book tenatively titled The Predators Within (TPW). TPW was to focus on phage and the human microbiome. As Breeann, Leah Pantea (illustrations), and I worked on TPW, it bacame clear that the science was still too nascent for a true synthesis. I decided that the best way forward, much to Breeann's chagrin, was to create

#### P.H.A.G.E.S. book

Read the book (pdf download, 48 MB)

Last updated: July 2, 2021

a synthesis of microbial ecology that would be the basis for TPW. P.H.A.G.E.S. is the result.Breeann and Leah are currently finishing the TPW.