V. Evolutionary Computing

B. Thermodynamics, Life & Evolution

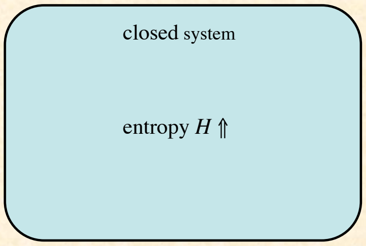
History vs. Science

- Historical question: *How did life emerge on earth?*
  - Knowledge of early conditions on earth is uncertain
  - Conditions differed in different locales
  - Precursors of life don't leave fossils
- Scientific question: *What physical processes can lead to the emergence of life?*
  - Studies the emergence of life in general
  - Develops scientific hypotheses about processes leading to emergence of life
  - Empirically confirms or disconfirms these hypotheses

Thermodynamics and Self-organization

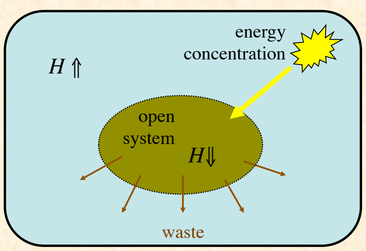
- *Macrostates* vs. *microstates*, and macroscopically indistinguishable microstates
- *Order*: macroscopic properties can be used to predict microscopic properties
- There are many more ways to be disordered than to be ordered
- The macrostate follows the most probable trajectory
- In the thermodynamic limit, the *likely* becomes *inevitable*, and the *unlikely, impossible*
- *Second Law*: an isolated system approaches the most likely (maximum entropy) macrostate
- *Maximum entropy principle*: an open system follows the most likely (maximum entropy producing) trajectory (controversial)

The Second Law of Thermodynamics



4/14/15 4

The Second Law and Open Systems



4/14/15 5

Nonequilibrium Thermodynamics

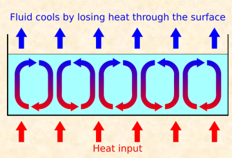
- Classical thermodynamics limited to systems in equilibrium
- Extended by thermodynamics of *transport processes*
  - i.e. accounting for entropy changes when matter/energy transported into or out of an *open system*
- Flow of matter/energy can maintain a *dissipative system* far from equilibrium for long periods
- Hence, *nonequilibrium thermodynamics*

4/14/15 6

An Energy Flow Can Create Structure

4/14/15 (photo from Camazine & al. *Self-Org. Bio. Sys.*) 7

Bénard Convection Cells



4/14/15 (photo from Camazine & al. *Self-Org. Bio. Sys.*, fig. from wikipedia) 8

Persistent Nonequilibrium Systems

- *If* flow creates system so structured to maintain flow
- *then* positive feedback causes nonequilibrium (NE) system to persist indefinitely
  - but not forever (2^{nd} law)
- Systems we tend to see are those most successful at maintaining NE state
- Applies to species as well as organisms

4/14/15 9

"Nature abhors a gradient"

— Eric D. Schneider

4/14/15 10

Selection Among Dissipative Systems

- If in a population some systems are more capable of converting free energy to entropy than others,
- then they will consume a higher fraction of the available free energy.
- Some systems get more free energy because they can use more free energy.

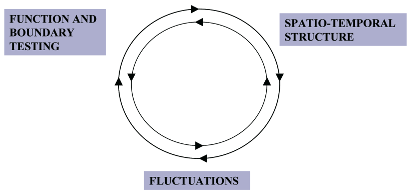
4/14/15 11

Decreased Internal Entropy

- Increasing the energy gradient forces the NE system to new states and modes, some of which may have a greater capacity to reduce the gradient.
  - bifurcations, symmetry breaking
    - far-from equilibrium system
- NE systems can increase capacity to accept free energy by using it to decrease internal entropy

4/14/15 12

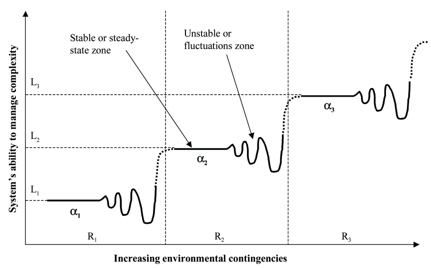
Order Through Fluctuations



- Fluctuations (esp. when system forced out of ordinary operating range) test boundaries & nonlinear effects
- May lead to stabilization of new structures

4/14/15 fig. < Hart & Gregor, *Inf. Sys. Found.* 13

Stratified Stability: Higher Levels of Organization



4/14/15 fig. < Hart & Gregor, *Inf. Sys. Found.* 14

Autocatalytic Processes

- Autocatalytic (self-reinforcing) processes may arise
  - stable cyclic behavior
    - attractor basins, bifurcations, chaos
  - growth and proliferation
    - access to new material & energy from environment

4/14/15 15

Selection

- Nonlinearities can lead to abrupt selection between more and less successful gradient reducers
- Small advantages can trigger rapid evolution
  - exponential selection

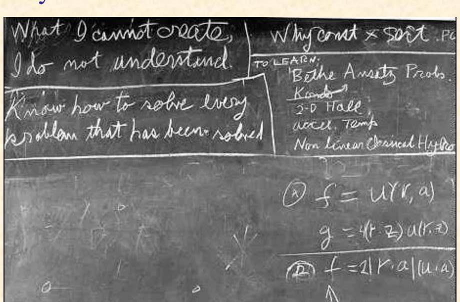
4/14/15 16

Storage

- NE systems may use generated internal structure (negentropy) to store material and energy
- thus maintaining a constant rate of entropy production in spite of fluctuations in external energy
  - immediate dissipation deferred to create internal gradients

4/14/15 17

Feynman's Blackboard When He Died



4/14/15 18

Building Blocks of Life

- Ingredients:
  - Hydrogen cyanide
  - Hydrogen sulfide
  - Ultraviolet light
- Leads to:
  - Nucleic acids (for RNA, DNA)
  - Amino acids (for proteins)
  - Lipids (for cell membranes)
- Source: *Science* (20 Mar. 2015) reporting on Sutherland et al. in *Nature Chemistry*

4/14/15 19

Dynamic Kinetic Stability

- Static stability
  - Thermodynamic stability
  - Less reactive
  - Kinetic barriers
  - Convergent ⇒ uniformity
- Dynamic stability
  - System is stable, not components
  - More reactive
  - Growth balanced by decay
  - Divergent ⇒ diversity

4/14/15 20

Replicating RNA

- In presence of enzyme (1967)
- Without enzyme (1986)
- RNA can function as enzyme (1989)
- Mutation & kinetic selection (1967)
- Simplification
  - 4000 nt to 550 nt

4/14/15 21

Competition

- Competitive Exclusion Principle (biology)
  - "Complete competitors cannot exist"
  - "Ecological differentiation is the necessary condition for coexistence"
- Competition among RNAs
  - Compete for same substrate ⇒ faster wins
  - Use different substrates ⇒ can coexist
  - Variety of usable substrates ⇒ evolve to use different substrates
  - Emergence of diversity (complexification of population)

Cooperation

- Investigation of RNA replication (Joyce, 2009)
- Single-RNA system: doubles in 17 hr
- Two-RNA system: doubles in 1 hr
  - Each produces the other
- Network formation
- More complex system can be faster replicator
- Greater dynamic kinetic stability

Emergence of Metabolism

- Molecule mutates to capture energy
- Demonstrated by simulation (2010)
- Activates building blocks so more reactive
- Increases dynamic kinetic stability
- Increases freedom from 2nd Law

What is Life?

- Basis of evolution:
  replication ⇒ mutation ⇒ complexification ⇒ selection ⇒ evolution
- Definition of life: "a self-sustaining kinetically stable dynamic reaction network derived from the replication reaction" (Pross, 2012, p. 164)

4/14/15 25

Life

- Life and other complex systems exist because of the 2^{nd} Law.
- They reduce pre-existing gradients more effectively than would be the case without them.
- Living systems optimally degrade energy for: growth, metabolism, reproduction.

4/14/15 26

Biological Organization

- "Entropic dissipation propels evolutionary structuring; nature's forces give it form." (Wicken)
- The simple-looking gradient represents potential complexity.
- "Order for free": the complexity of organisms is always paid for by the richness of pre-existing gradients.

4/14/15 27

"Order for Free"

- Relatively simple sets of rules or equations can generate rich structures & behaviors
- Small changes can lead to qualitatively different structures & behaviors
- A diverse resource for selection
- A basis for later fine tuning (microevolution)
- See Kaufmann (*At Home in the Universe*, etc.) and Wolfram (*A New Kind of Science*)

Thermodynamic Selection

- "Even before natural selection, the second law 'selects' from the kinetic, thermo-dynamic, and chemical options available those systems best able to reduce gradients under given constraints." (Schneider)
- "Natural selection favors systems adept at managing thermodynamic flows." (ibid)

Evolution of Species

- Evolution proceeds in such a direction as to make the total energy flux through the system a maximum compatible with the constraints.
- But organisms and species must also channel energy toward the preservation and expansion of themselves as material systems.

Ecosystem Evolution

- Ecosystems evolve in the way they handle energy:
- Earlier:
  - fast growth
  - more similar units
- Later:
  - slower growth
  - more diversity

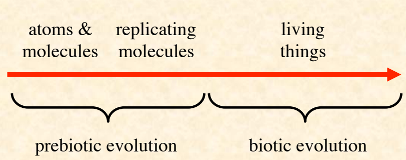
4/14/15 31

Evolution in Broad Sense

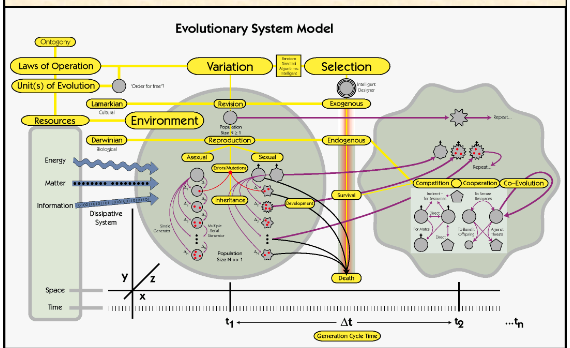
- Evolution in the broadest terms:
  - blind variation
  - selective retention
- Has been applied to nonbiological evolution
  - evolutionary epistemology
  - creativity
  - memes

4/14/15 32

Evolution



4/14/15 33



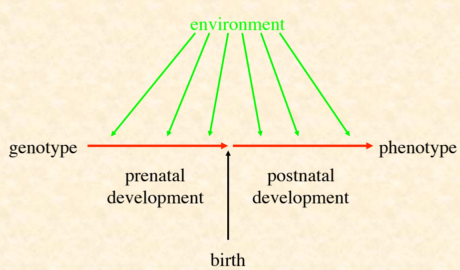
4/14/15 (from NECSI) 34

Genotype vs. Phenotype

- Genotype = the genetic makeup of an individual organism
- Phenotype = the observed characteristic of the organism
- Through interaction with environment, a genotype is *expressed* in a phenotype

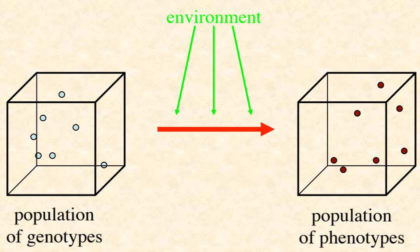
4/14/15 35

Ontogeny



4/14/15 36

Genotype Space vs. Phenotype Space



Selection

- Selection operates on the phenotype, not the genotype
- Selection of genotypes is indirect

"Central Dogma" of Genetics

- "The transfer of information from nucleic acid to nucleic acid, or from nucleic acid to protein may be possible, but transfer from protein to protein, or from protein to nucleic acid is impossible."
  – Francis Crick
- A hypothesis (not a dogma)
- "New" Lamarckism: "jumping genes" and reverse transcription

Essentialism vs. "Population Thinking"

- Essentialism: each species has a fixed, ideal "type"
  - actual individuals are imperfect expressions of this ideal
  - species have sharp boundaries
  - the type is real, variation is "illusory" (secondary)
- Population thinking: a species is a reproductive population
  - only individual organisms exist
  - species have blurred boundaries
  - species are time-varying "averages"
  - variation is real, the type is an abstraction

4/14/15 40

Fitness

- 1st approximation: the relative ability of an individual organism to optimize the energy flow to maintain its nonequilibrium state long enough to reproduce (survival fitness)
- 2nd approximation: reproductive fitness = the relative efficiency at producing viable offspring
  - of oneself (exclusive fitness)
  - of oneself or close relatives (inclusive fitness)

4/14/15 41

"Selfish Gene"

- An organism is a gene's way of making more copies of itself
- A gene (or collection of genes) will tend to persist in a population if they tend to produce physical characteristics & behavior that are relatively successful at producing more copies of itself
- Nevertheless, it is physical organisms (phenotypes) that confront the environment

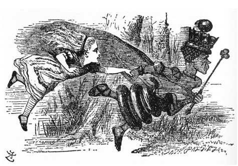
4/14/15 42

Complicating Factors

- Individual genes influence multiple characteristics & behaviors
- Genes are not independent
- "Fitness" is in the context of a (possibly changing) environment including:
  - conspecifics
  - coevolving predators and prey
- Conclusion: beware of oversimplifications
  - keep entire process in mind

4/14/15 43

The Red Queen Hypothesis



"Now, *here*, you see, it takes all the running *you* can do, to keep in the same place."
— *Through the Looking-Glass and What Alice Found There*

- *Observation*: a species probability of extinction is independent of time it has existed
- *Hypothesis*: species continually adapt to each other
- Extinction occurs with insufficient variability for further adaptation

4/14/15 44

Can Learning Guide Evolution?

- "Baldwin Effect":
  - proposed independently in 1890s by Baldwin, Poulton, C. Lloyd Morgan
  - spread of genetic predispositions to acquire certain knowledge/skills
- Gene-culture coevolution
- Special case of *niche construction*: organisms shape the environments in which they evolve
- Also involves *extragenetic inheritance*
- Indirect causal paths from individual adaptation to genome

4/14/15 45

Example Effects of Single Genes

4/14/15 46

Butterfly Eyespots

- Major changes within 6 generations
- May lead to patterns not seen in previous generations

4/14/15 (photos from *Science* 1 Nov 2002) 47

Two Populations of *Astyanax mexicanus*

- Two populations of one species
- Regulation of one gene (controlling head development)
  - eyes, smaller jaws, fewer teeth
  - blind, larger jaws, more teeth

4/14/15 (photos from *Science* 1 Nov 2002) 48

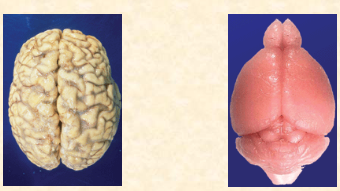
Human Fear Response

(photos from *Science* 19 July 2002)

Single Gene Affecting Human Fear Response

- Two alleles for gene:
  - short allele $\Rightarrow$ greater anxiety response to angry or frightened faces
  - long allele $\Rightarrow$ lesser response
- Gene encodes transporter protein, which carries serotonin back into neuron after release
- Short allele produces 1/2 amount of protein
- Accumulating serotonin affects neighboring cells

Human vs. Rat Cortex



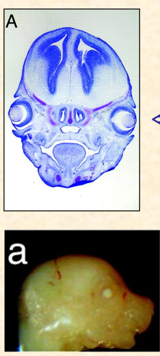
- Human cortex relatively larger
- Also more structured

Experiment

- Problem: How do organs know when to stop growing?
- Genetically engineer rats to express a mutant form of protein (β-catenin)
- More resistant to breakdown, ∴ accumulates
- Spurs neural precursor cells to proliferate

4/14/15 52

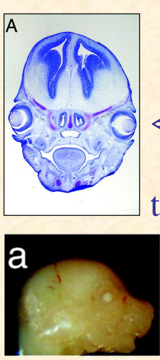
Results



⇐ normal

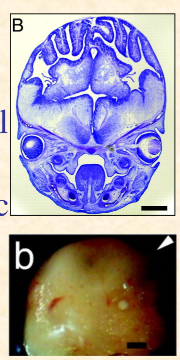
4/14/15 (photos from Chenn & Walsh 2002) 53

Results



⇐ normal

transgenic ⇒



4/14/15 (photos from Chenn & Walsh 2002) 54

Why are Our Brains Bigger than Chimp Brains?

- Genes controlling NK white blood cells differ slightly between humans & chimps
- Chimp NK cells give them immunity to HIV, malaria, etc.
- But NK cells also control blood-flow to the fetus
- In humans, it is critical that the fetus have an adequate blood supply for its large brain
- Studies suggest NK cells can be optimized for one or the other, not both
- Peter Parham (Stanford): Abi-Rached, Moesta, Rajalingam, Guethlein, Parham (2010), *PLoS Genetics* 6 (11): e1001192. doi:10.1371/journal.pgen.1001192

4/14/15 55

Additional Bibliography

1. Goldberg, D.E. *The Design of Innovation: Lessons from and for Competent Genetic Algorithms*. Kluwer, 2002.
2. Milner, R. *The Encyclopedia of Evolution*. Facts on File, 1990.
3. Pross, A. *What is Life: How Chemistry Becomes Biology*. Oxford, 2012.
4. Schneider, E.D., & Sagan, D. *Into the Cool: Energy Flow, Thermodynamics, and Life*. Chicago, 2005.

4/14/15 56