CS 790R Seminar
Modeling & Simulation

Computational Models of Complex Systems

~ Introductory Lecture 2 ~

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Computational Models of Complex Systems

Introductory Lecture 1

- Examples of complex systems 1
- Course organization
- Paper reviews (first period)

Introductory Lecture 2

- Examples of complex systems 2
- Common elementary features of CS
- Common global properties of CS

Computational Models of Complex Systems

Introductory Lecture 2

- Examples of complex systems 2
  - Pattern formation
  - Insect colonies
  - Group motion
  - Synchronization
- Common elementary features of CS
- Common global properties of CS

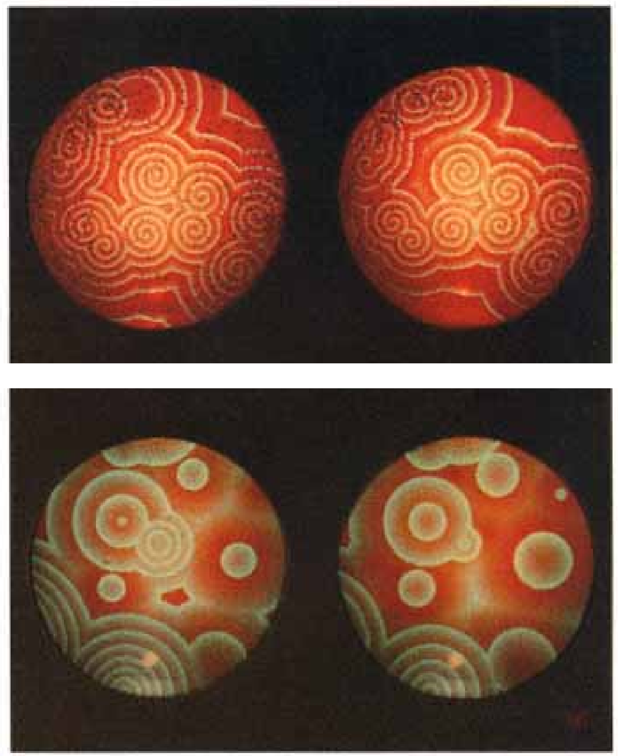
Computational Models of Complex Systems

Introductory Lecture 2

- Examples of complex systems 2
  - Pattern formation
    - Physical: convection cells
    - Chemical: BZ reaction
    - Biological: animal colors
    - Biological: slime mold
  - Insect colonies
  - Group motion
  - Synchronization
- Common elementary features of CS
- Common global properties of CS

Examples of complex systems
Pattern formation – *Chemical: BZ reaction*

4-second oscillations of the BZ reaction in a well-stirred tank
(Gabriel Peterson, College of the Redwoods, CA)

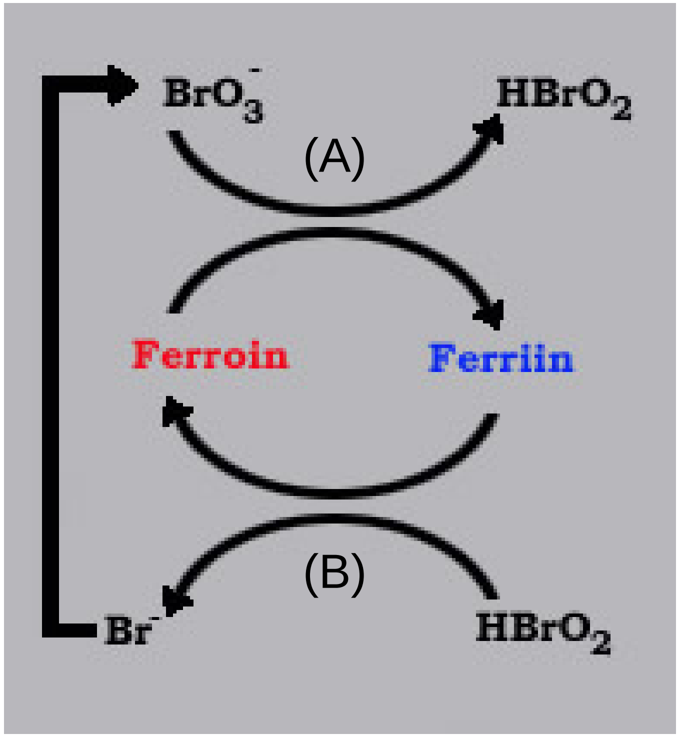


Spiral and circular traveling waves of the BZ reaction in a Petri dish
(Arthur Winfree, University of Arizona)

Phenomenon

- Belousov-Zhabotinsky reaction: “chemical clock”
- if well stirred, it oscillates
- if spread on a plate, it creates waves (reaction-diffusion)
- example of an “excitable medium”
- often cited in self-organization

Examples of complex systems
Pattern formation – *Chemical: BZ reaction*



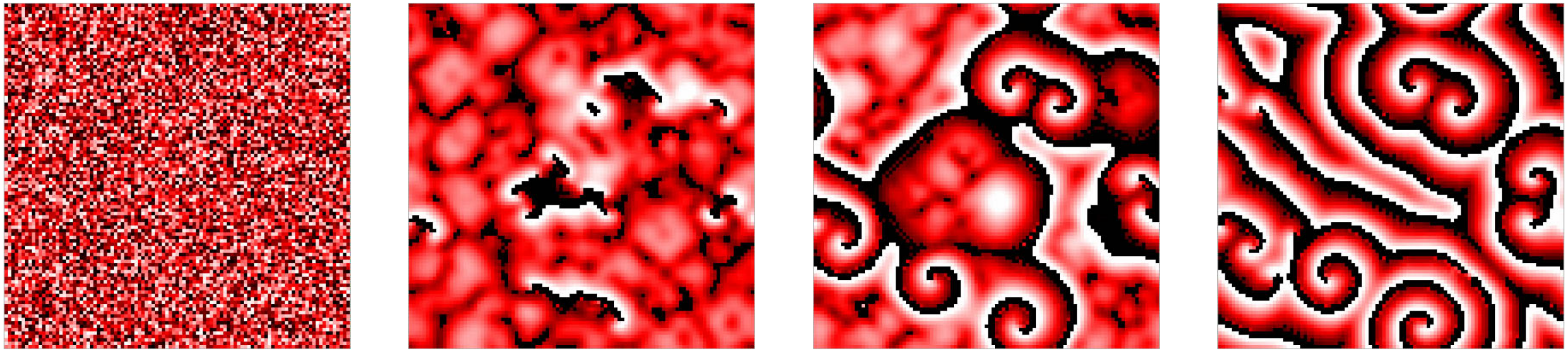
Simplified diagram of the Belousov-Zhabotinsky reaction
(Gabriel Peterson, College of the Redwoods, CA)

Mechanism

- competition between two reaction branches, A and B
- A is faster than B, but B is autocatalytic
- when A runs out of reactants, B takes over and regenerates them
- a color indicator signals the switch between A and B through iron ions (Fe^{2+}/Fe^{3+})

Examples of complex systems

Pattern formation – *Chemical: BZ reaction*



NetLogo B-Z reaction simulation, after A. K. Dewdney's "hodgepodge machine"
(Uri Wilensky, Northwestern University, IL)

Modeling & simulation

- abstract, simplified rules
- each cell has 3 states:
  - "healthy" (x = 0, black)
  - "infected" (0 < x < 1, red)
  - "sick" (x = 1, white)

- each cell follows 3 rules:
  - if "sick", become "healthy"
  - if "healthy, become "infected" as a function of neighbors
  - if "infected", increase infection level as a function of neighbors

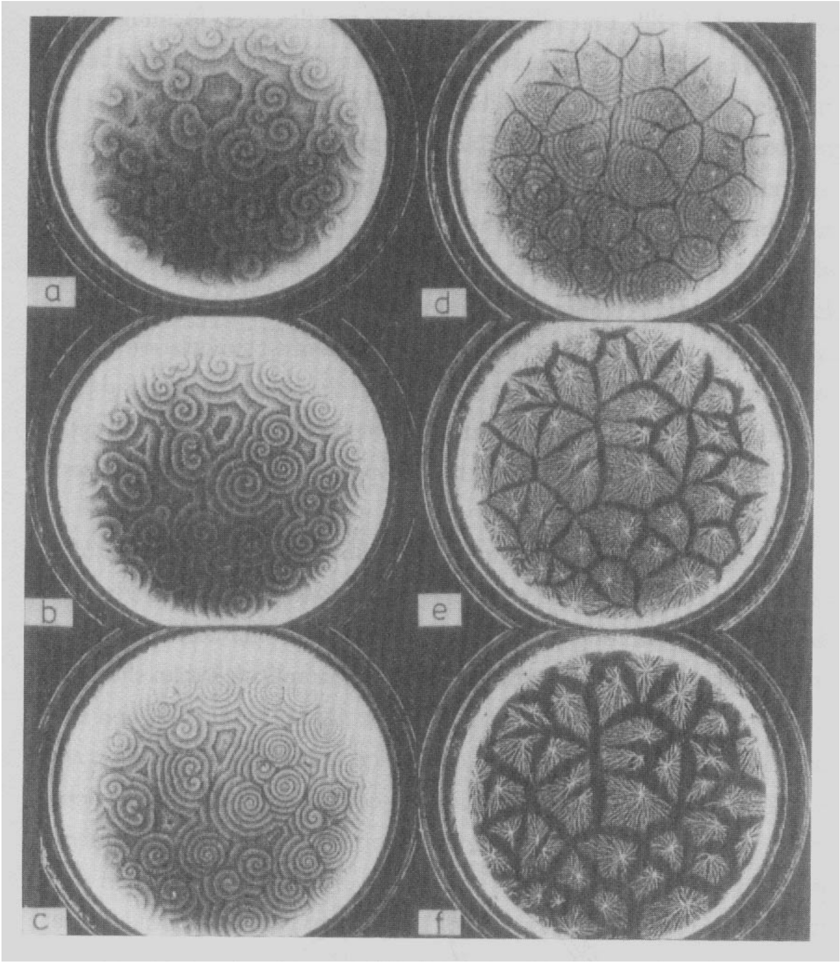
Examples of complex systems

Pattern formation – *Chemical: BZ reaction*

Concepts collected from this example

- simple individual rules (modeling a less simple, but small set of reactions)
- emergence of long-range spatiotemporal correlations
- no impurities; spiral centers are *not* specialized (decentralization)
- local interactions by reaction and diffusion

Examples of complex systems
Pattern formation – *Biological: slime mold*

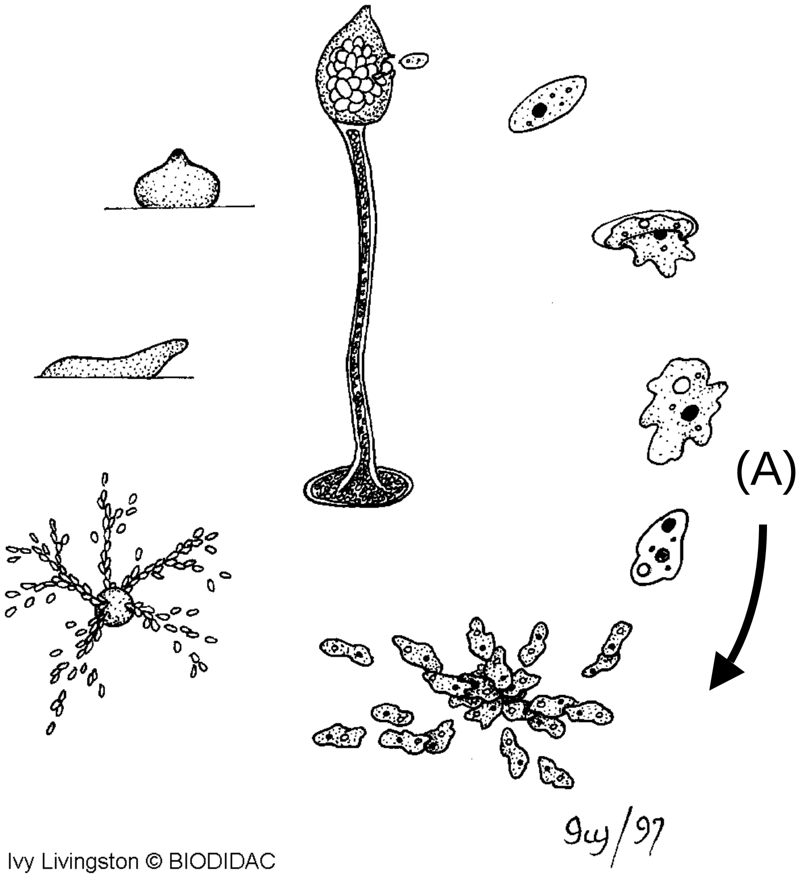


Synchronization, breakup and aggregation of slime mold amoebae on an agar plate
(P. C. Newell; from Brian Goodwin, "How the leopard changed its spots", Princeton U. Press)

Phenomenon

- unicellular organisms (amoebae) clump together into multicellular "slugs"
- with enough food, they grow and divide independently
- under starvation, they synchronize (chemical waves), aggregate and differentiate
- aggregation phase shows same concentric wave patterns as BZ reaction
- another famous example of "excitable medium" and self-organization

Examples of complex systems
Pattern formation – *Biological: slime mold*



Life cycle of Dictyostelium slime mold
(Ivy Livingstone, BIODIDAC, University of Ottawa)

Mechanism

- life cycle of slime mold amoebae (Dictyostelium):

  independent amoebae (A)

  → aggregation

  → clump

  → slug

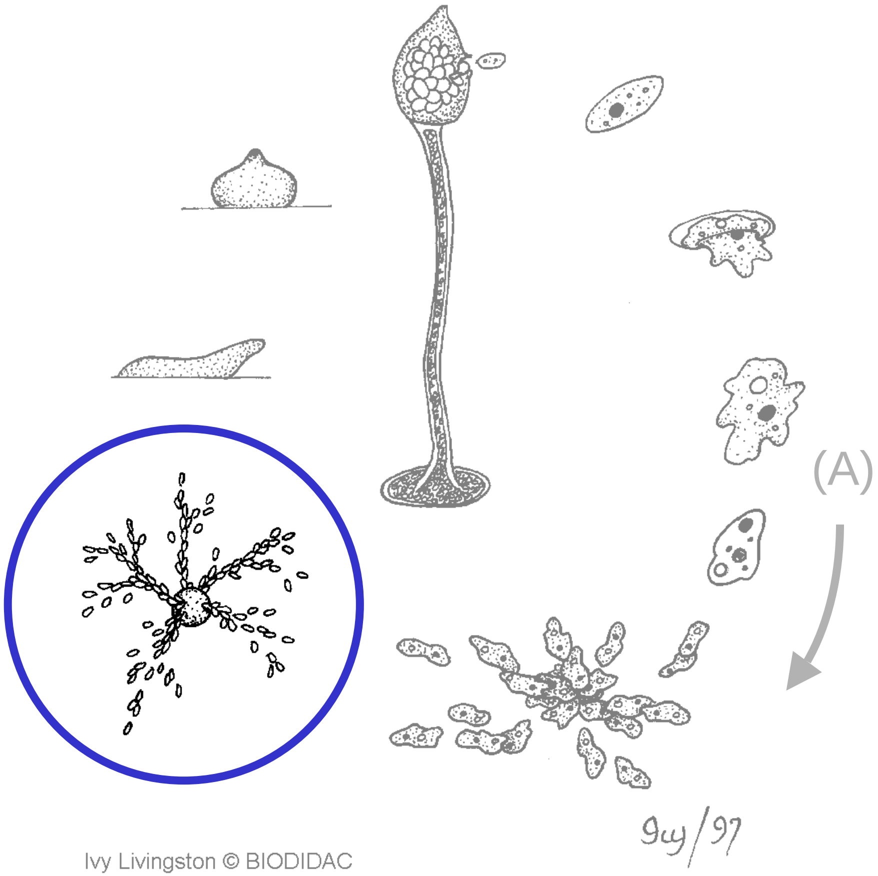
  → growth

  → body & fruit

  → spore release & germination

  → amoebae (A)

Examples of complex systems
Pattern formation – *Biological: slime mold*



Life cycle of Dictyostelium slime mold
(Ivy Livingstone, BIODIDAC, University of Ottawa)

Mechanism

- life cycle of slime mold amoebae (Dictyostelium):

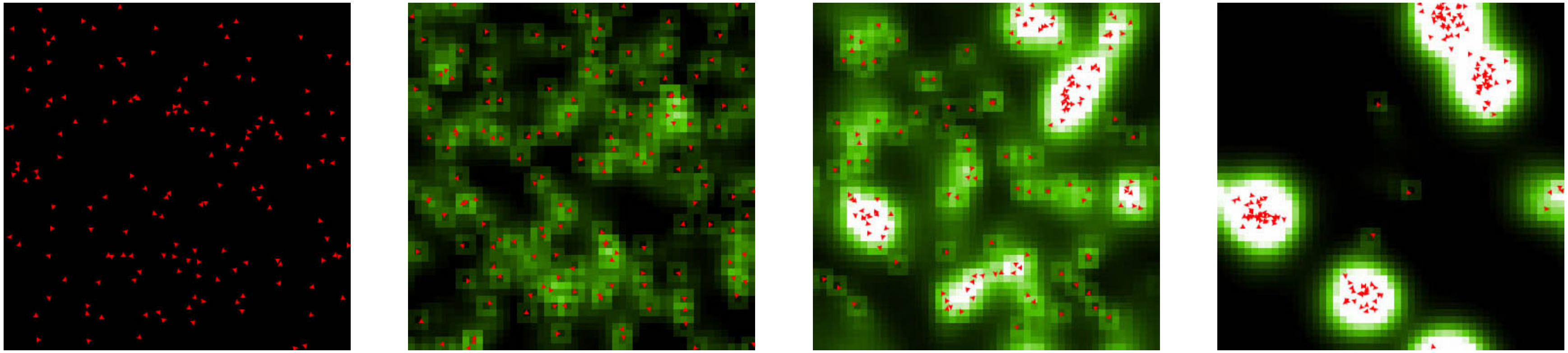
  independent amoebae (A)

  → aggregation
  - stage 1: oscillatory secretion of chemical (cAMP) by each cell
  - stage 2: local coupling of secretion signal, forming spiral waves
  - stage 3: pulsatile motion toward spiral centers

  → clump

  → ...

Examples of complex systems
Pattern formation – *Biological: slime mold*



NetLogo simulation of slime mold aggregation, after Mitchel Resnick
(Uri Wilensky, Northwestern University, IL)

Modeling & simulation

- for wave formation (stages 1 & 2 of aggregation)

  → *see B-Z reaction model*

- for clumping (stage 3 of aggregation), three simplified rules:
  - each cell (red) secretes a chemical (shades of green)
  - each cell moves towards greater concentration of chemical
  - chemical evaporates

Examples of complex systems
Pattern formation – *Biological: slime mold*

Concepts collected from this example

- simple, "blind" individual behavior
- emergence of aggregates
- spiral centers are *not* already differentiated cells (decentralization)
- local interactions (cell $\leftrightarrow$ chemical)
- phase transition (critical mass)

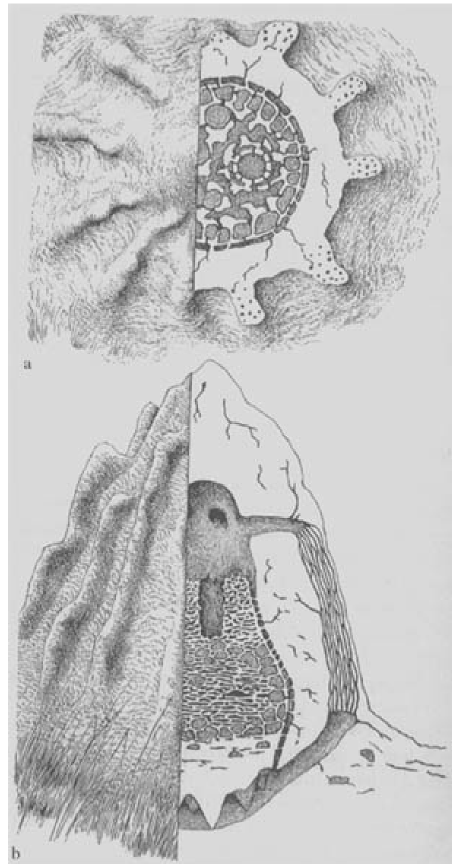
Computational Models of Complex Systems

Introductory Lecture 2

- Examples of complex systems 2
  - Pattern formation
  - Insect colonies
    - Ant trails
    - Termite mounds
  - Group motion
  - Synchronization
- Common elementary features of CS
- Common global properties of CS

Examples of complex systems
Insect colonies – *Termite mounds*

Termite mound
(J. McLaughlin, Penn State University)

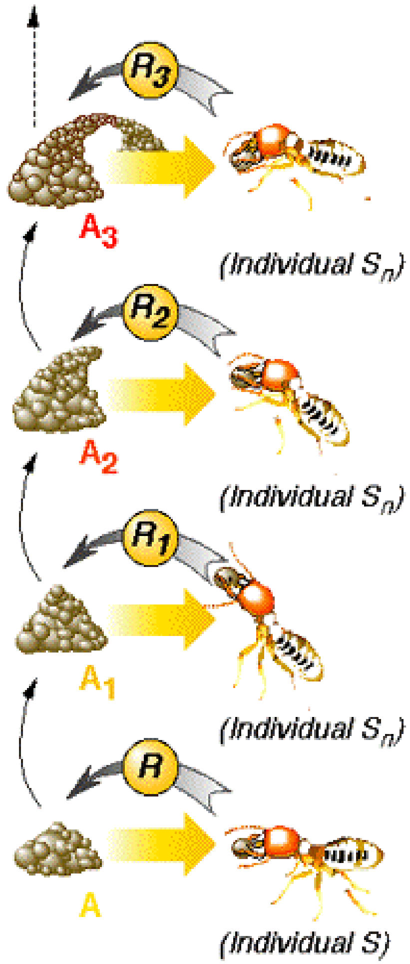


Inside of a termite mound
(Lüscher, 1961)

Phenomenon

- another example of insect self-organization: mound building by termites
- remarkable size and detailed architecture
- essentially made of tiny pellets of soil glued together
- starts with one underground chamber and grows up like a plant

Examples of complex systems
Insect colonies – *Termite mounds*



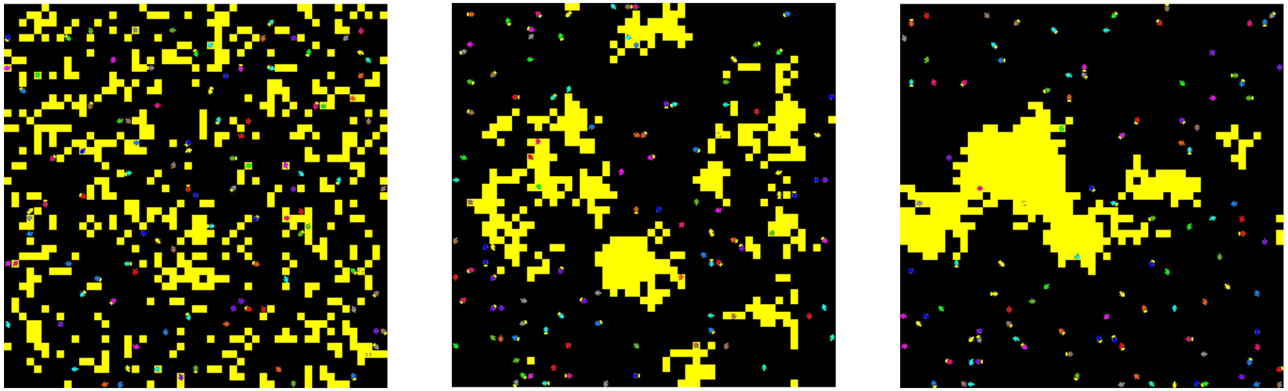
Termite stigmergy

(after Paul Grassé; from Solé and Goodwin, "Signs of Life", Perseus Books)

Mechanism

- no plan or central control
- termites do not interact directly but rather indirectly, through the environment they are modifying
- "stigmergy" is a set of stimulus-response pairs:
  - pattern A in environment triggers behavior R in termite
  - behavior R changes A into A_1
  - pattern A_1 triggers behavior R_1
  - behavior R_1 changes A_1 into A_2
  - etc.
- for example, a small heap develops into an arch

Examples of complex systems
Insect colonies – *Termite mounds*



StarLogo termite mound building simulation, after Mitchel Resnick
(StarLogo Project, MIT Media Laboratory, MA)

Modeling & simulation

- simplified setup:
  - randomly scattered wood chips (or soil pellets)
  - termites moving among the chips
- virtual termite's repertoire:
  - walk around randomly
  - if bump into wood chip, pick it up and move away
  - if carrying wood chip, drop it where other wood chips are
- result: wood chips are stacked in piles of growing size
- explains one aspect of mound formation

Examples of complex systems
Insect colonies – *Termite mounds*

Concepts collected from this example

- simple individual rules
- emergence of macroscopic structure
- no architect, no blueprint
- amplification of small fluctuations (positive feedback)
- local interactions (termite $\leftrightarrow$ environment)

Computational Models of Complex Systems

Introductory Lecture 2

- Examples of complex systems 2
  - Pattern formation
  - Insect colonies
  - Group motion
    - Natural: flocks, schools, herds
    - Artificial: traffic jams
  - Synchronization
- Common elementary features of CS
- Common global properties of CS

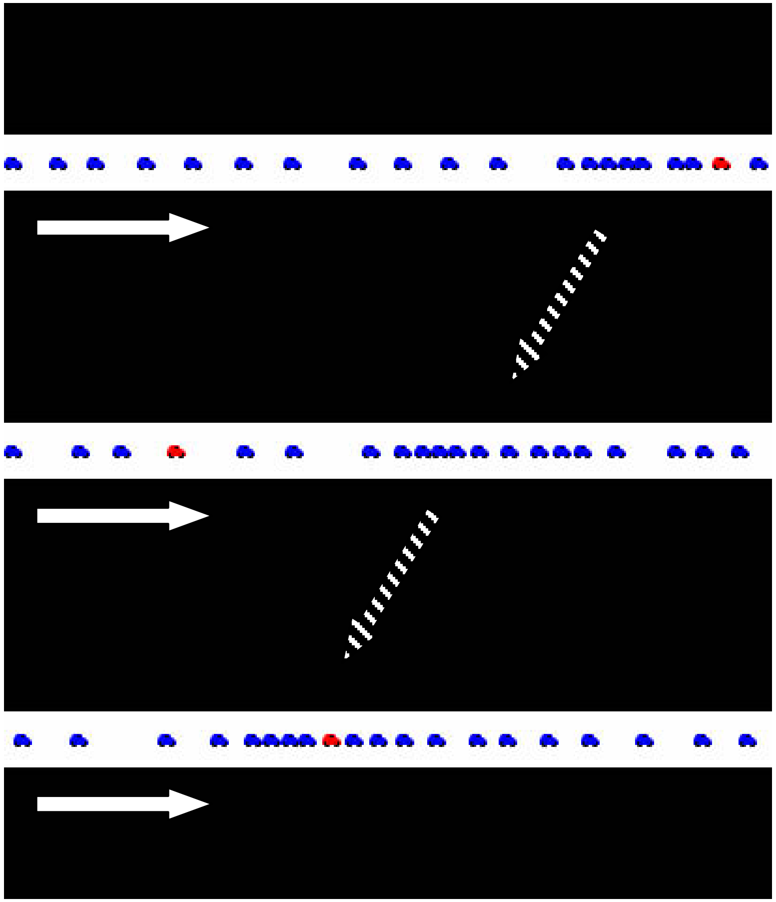
Examples of complex systems
Group motion – *Artificial: traffic jams*

Traffic jam
(Department of Physics, University of Illinois at Urbana-Champaign)

Phenomenon

- stream of cars breaks down into dense clumps and empty stretches
- spontaneous symmetry-breaking of initially uniform density and speed
- no need for a central cause (slow vehicle, stop light or accident)

Examples of complex systems
Group motion – *Artificial: traffic jams*



NetLogo traffic basic simulation, after Mitchel Resnick
(Uri Wilensky, Northwestern University, IL)

Modeling & simulation

- each car:
  - slows down if there is another car close ahead
  - speeds up if there is no car close ahead
- traffic nodes move in the direction opposite to cars
- emergence of group behavior qualitatively different from individual behavior

Examples of complex systems
Group motion – *Artificial: traffic jams*

Concepts collected from this example

- simple individual reactions
- emergence of moving superstructures
- no accident, no light, no police radar (decentralization)
- amplification of small fluctuations (positive feedback)
- local interactions (car $\leftrightarrow$ car)

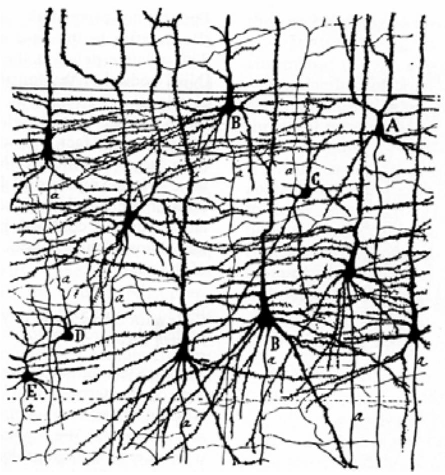
Computational Models of Complex Systems

Introductory Lecture 2

- Examples of complex systems 2
  - Pattern formation
  - Insect colonies
  - Group motion
  - Synchronization
    - Fireflies
    - Neurons
- Common elementary features of CS
- Common global properties of CS

Examples of complex systems
Synchronization – *Neurons*

Medial surface of the brain
(Virtual Hospital, University of Iowa)

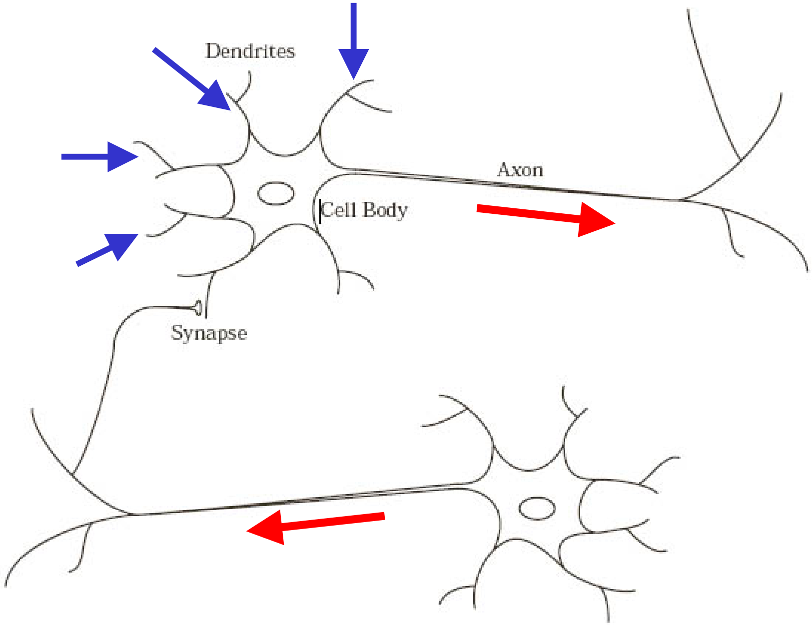


Pyramidal neurons and interneurons, precentral gyrus
(Ramón y Cajal 1900)

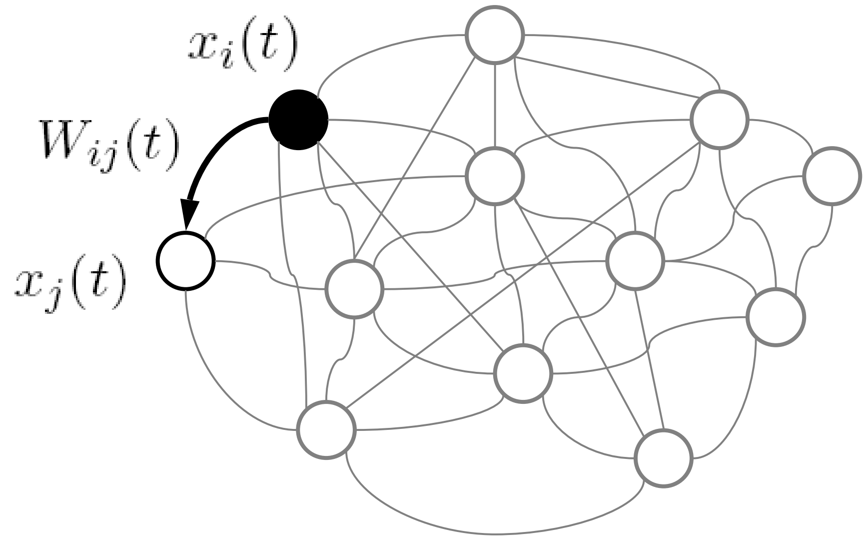
Phenomenon

- neurons together form... the brain! (+ peripheral nervous system)
  - perception, cognition, action
  - emotions, consciousness
  - behavior, learning
  - autonomic regulation: organs, glands
- ~10^{11} neurons in humans
- communicate with each other through electrical potentials
- neural activity exhibits specific patterns of *spatial and temporal synchronization* (“temporal code”)

Examples of complex systems
Synchronization – *Neurons*



Schematic neurons
(adapted from CS 791S "Neural Networks", Dr. George Bebis, UNR)



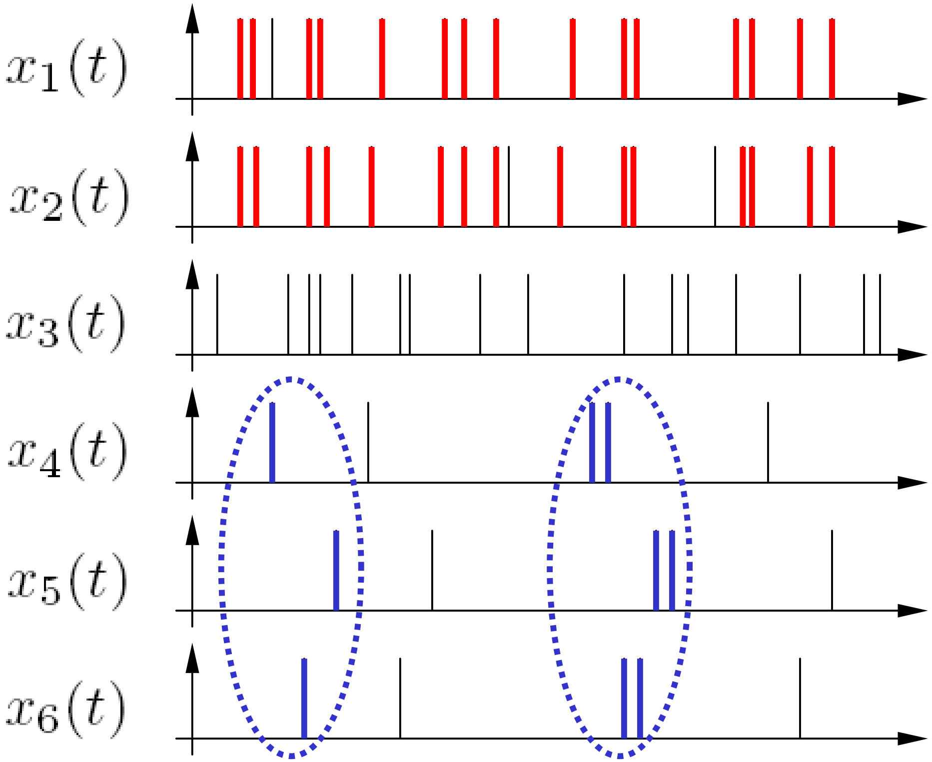
A binary neural network

Mechanism

- each neuron receives signals from many other neurons through its *dendrites*
- the signals converge to the *soma* (cell body) and are integrated
- if the integration exceeds a threshold, the neuron fires a signal on its *axon*

Examples of complex systems

Synchronization – *Neurons*



$\langle x_1(t) \rangle =$ ● high activity rate

$\langle x_2(t) \rangle =$ ● high activity rate

$\langle x_3(t) \rangle =$ ● high activity rate

$\langle x_4(t) \rangle =$ ○ low activity rate

$\langle x_5(t) \rangle =$ ○ low activity rate

$\langle x_6(t) \rangle =$ ○ low activity rate

$$\langle x_1(t)\, x_2(t) \rangle \gg \langle x_1(t)\, x_3(t) \rangle$$

- 1 and 2 more in sync than 1 and 3

$$\langle x_4(t)\, x_5(t - \tau_{4,5})\, x_6(t - \tau_{4,6}) \rangle$$

- 4, 5 and 6 correlated through delays

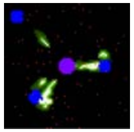
Computational Models of Complex Systems

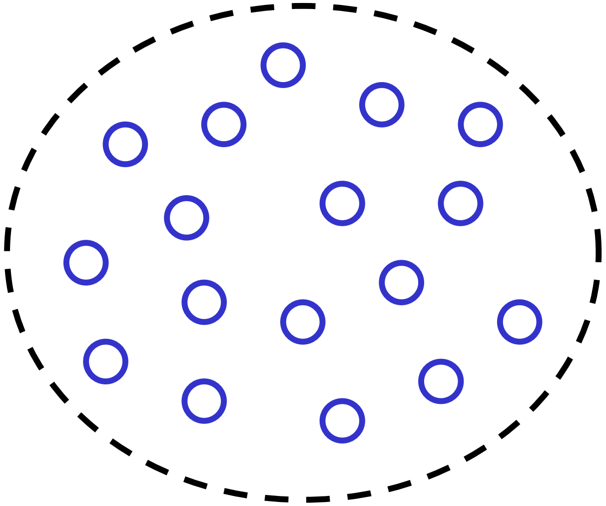
Introductory Lecture 2

- Examples of complex systems 2
- Common elementary features of CS
  - Large number of elements
  - Simple behavior rules
  - Local interactions
  - Network interactions
  - Hierarchy of levels
- Common global properties of CS

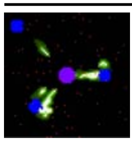
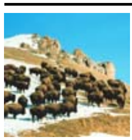
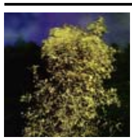
Common elementary features of CS

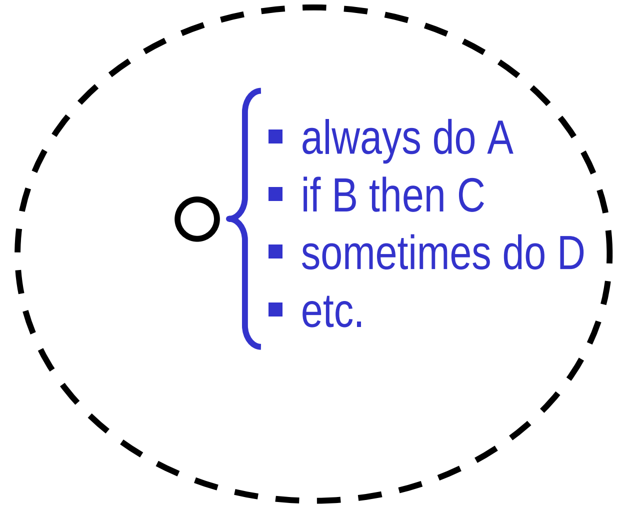
Large number of elements

	BZ reaction	*molecules*
	slime mold	*amoebae*
	animal coats	*embryo cells*
	insect colonies	*ants, termites, bees*
	flocking, traffic	*birds, fish, cars*
	synchronization	*fireflies, neurons*



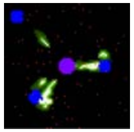
Common elementary features of CS
Simple behavior rules

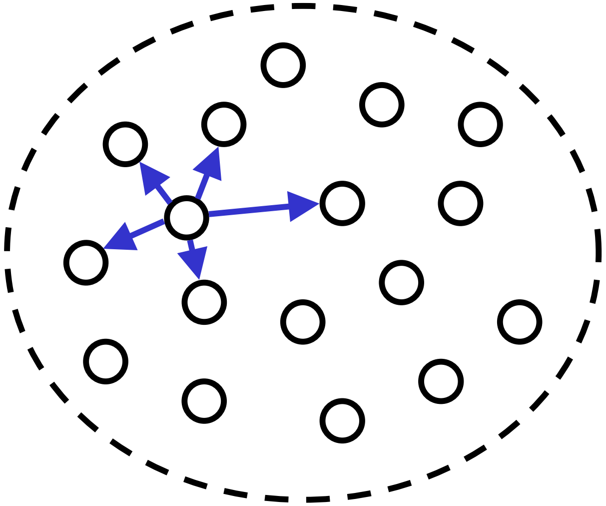
	BZ reaction	*react, diffuse*
	slime mold	*diffuse, sync, move*
	animal coats	*activate, inhibit*
	insect colonies	*carry, deposit, follow*
	flocking, traffic	*steer, adjust speed*
	synchronization	*reset phase/freq.*



- limited repertoire of fixed and reactive behavior
- elements are not *intrinsically* simple, only *functionally* at the level of description of the studied process

Common elementary features of CS
Local interactions

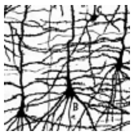
	BZ reaction	*molecular collisions*
	slime mold	*cAMP signaling*
	animal coats	*morphogens*
	insect colonies	*pheromone*
	flocking, traffic	*visual recognition*
	synchronization	*light/electric stimulus*

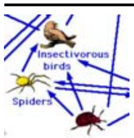


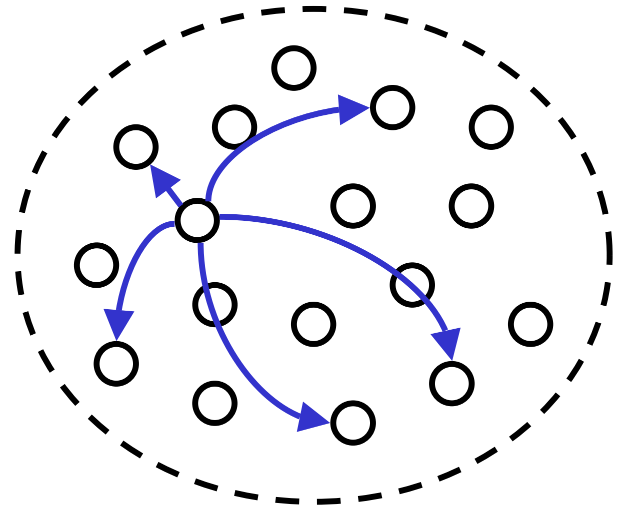
- each element interacts with other elements and/or the environment in a local neighborhood
- one-to-one or broadcast messaging

Common elementary features of CS

Network interactions

	(3-D space)	
	neurons	*axons*
	Internet, Web	*wires, hyperlinks*

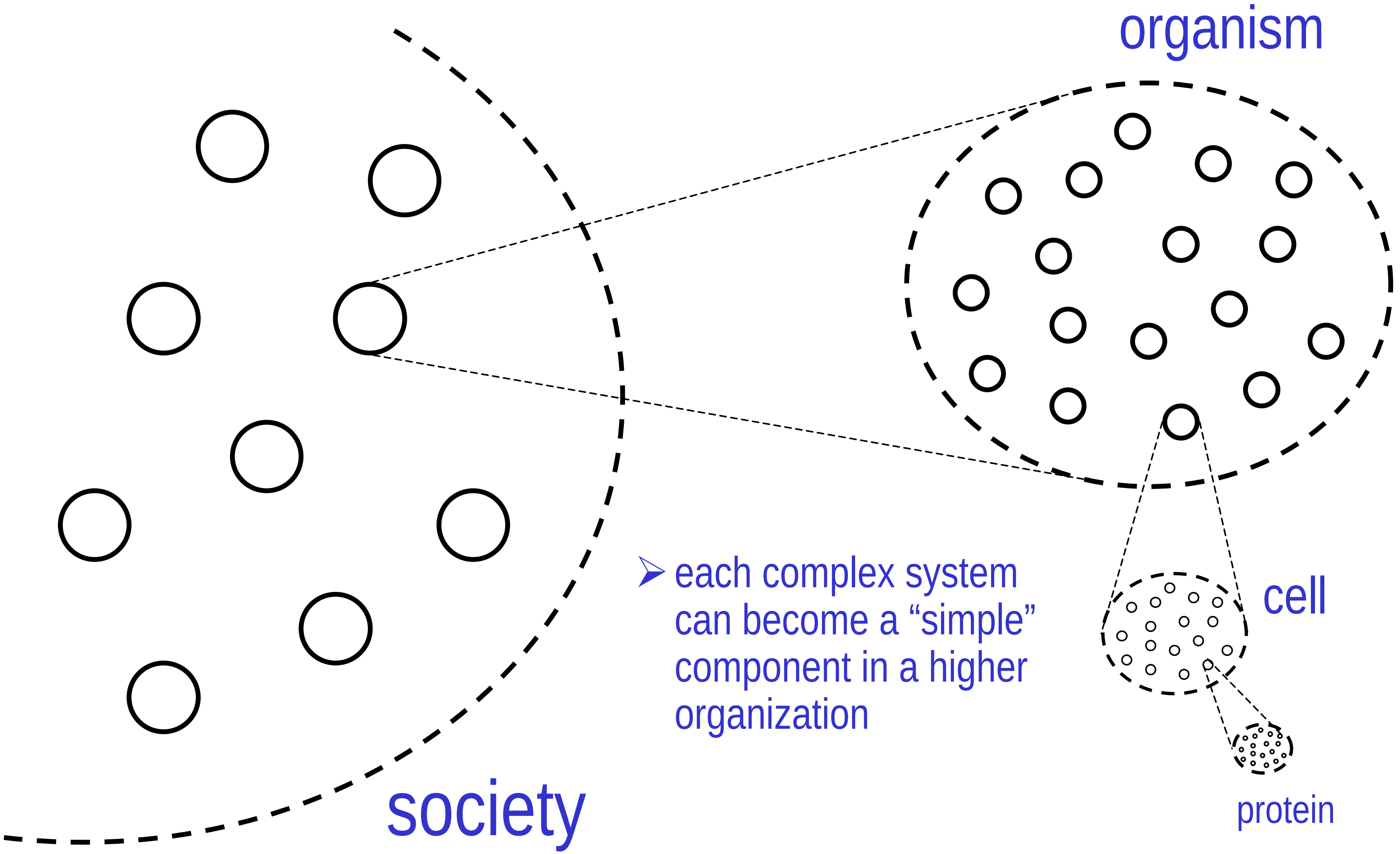
	(non-spatial)	
	gene network	*regulatory enzymes*
	food web	*predation*



- local neighborhood is not necessarily 2-D or 3-D, but also long-range graph...
- ... or *both*: “small worlds”
- also, non-spatial models: types, species

Common elementary features of CS

Hierarchy of levels



- each complex system can become a "simple" component in a higher organization

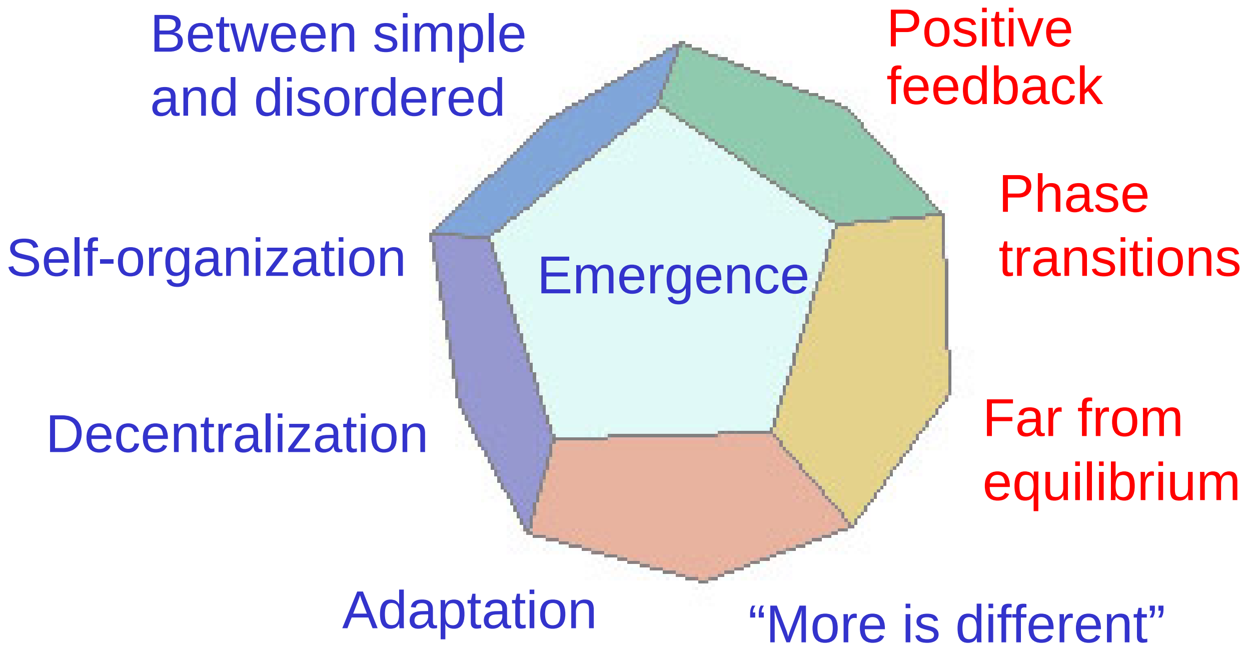
Computational Models of Complex Systems

Introductory Lecture 2

- Examples of complex systems 2
- Common elementary features of CS
- Common global properties of CS
  - Emergence
  - Self-organization
  - Decentralization
  - Between simple and disordered
  - “More is different”, phase transitions
  - Positive feedback
  - Far from equilibrium
  - Adaptation

Common global properties of CS

- ✓ key concepts (“buzzwords”) expressing different facets of CS:
  - some have different definitions across disciplines; no global agreement
  - others have a clearer meaning but different weights in “making” CS
  - terms overlapping but not equivalent; yet, often grouped or interchanged



Common global properties of CS
Emergence

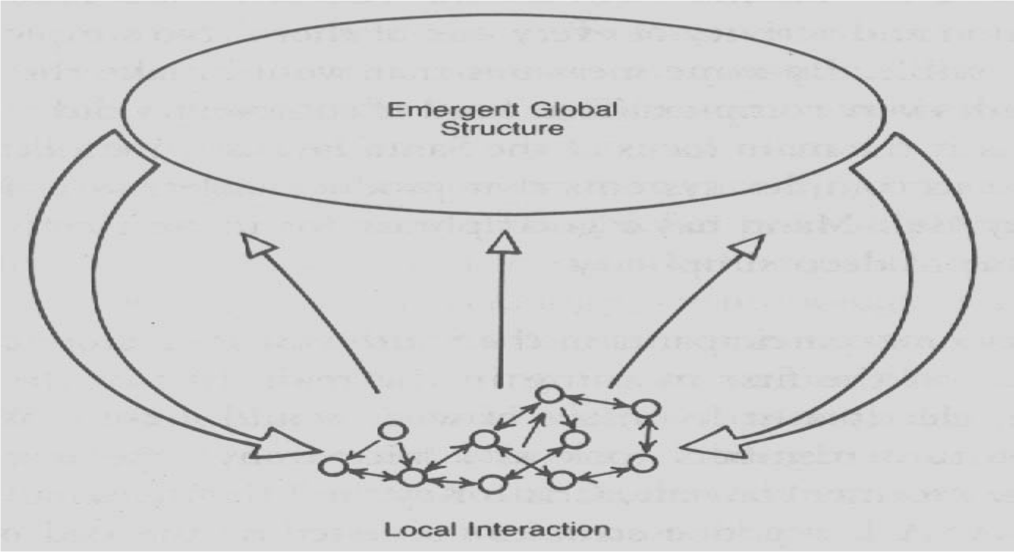
- ✓ the system has properties that the elements do not have
  - ex: macroscopic patterns from microscopic units (convection rolls, spiral waves, stripes, spots)
  - ex: intelligent collective decision making from “ignorant” individuals (insect colonies, neurons, market traders)
- ✓ these properties cannot be easily inferred or predicted
  - ex: liquid water or ice emerging from H_2O molecules
  - ex: cognition and consciousness emerging from neurons
- ✓ different properties can emerge from the same elements/rules
  - ex: the same molecules of water combine to form liquid or ice crystals
  - ex: the same cellular automaton rule changes behavior with initial state
- ✓ global properties can constitute local rules at a higher level: jumping from level to level through emergence

Common global properties of CS
Self-organization

- ✓ the organization or “order” of the system increases internally without external intervention
  - ex: aggregating processes (slime mold, pigmentation spots, termite heaps, flocks, etc.)
- ✓ order can be quantified using an “order parameter”
  - ex: cluster rate in aggregation
  - ex: long-range spatiotemporal correlations (spiral waves, synchrony)
- ✓ crucial to the notion of *self*-organization are the interactions *among* elements (vs. interaction with an external cause)
  - either directly: element ↔ element
  - or indirectly: element ↔ environment ↔ element (“stigmergy” in social insects)

Common global properties of CS
Emergence & Self-organization

- ✓ counter-examples of emergence *without* self-organization:
  - ex: well-informed leader (orchestra conductor, military officer)
  - ex: global plan (construction area), full instructions (orchestra)
- ✓ the emergent structure can also feed back to the elements
  - ex: market influences buyers, traffic jam influences drivers



Chris Langton's view of emergence in complex systems
(from "Complexity", Roger Lewin, University of Chicago Press)

Common global properties of CS
Decentralization

- ✓ order without a leader
  - ex: the central amoeba in spiral waves is *not* a pacemaker
  - ex: the queen ant is *not* a manager
  - ex: the first bird in a V-shaped flock is *not* a leader
- ✓ the “invisible hand”:
  - distribution: each element carry a small piece of the global information
  - ignorance: elements do not have explicit goals or intentions
  - parallelism: elements act simultaneously
- ✓ decentralized processes are far more abundant than leader-guided processes, in nature and human societies
- ✓ ... and yet, the notion of decentralization is still counterintuitive
  - many decentralized phenomena are still poorly understood
  - a “leader-less” or “designer-less” explanation still meets resistance

  → human perceptual bias toward an identifiable source or primary cause

Common global properties of CS
Between simple and disordered

- ✓ Warren Weaver's 1948 classification of scientific activity:
  1. **Problems of simplicity** 1- to 3-variable problems of the 17th, 18th and 19th centuries: Newtonian mechanics, electricity, chemistry, etc.
  2. **Problems of disorganized complexity** million- and billion-variable problems of the 20th century: statistical mechanics (gas, fluid, solid), probability theory, theory of information, etc.
  3. **Problems of organized complexity ("middle region")** dozens or hundreds of *interrelated* variables [21st century problems]: biology, medicine, psychology, economics, social science, etc.
- ✓ the billiards table analogy*
  1. a few balls: individual trajectories from velocities, angles, friction
  2. a million balls: only broad statistical trends (average path, pressure)
  3. a hundred motorized balls obeying simple rules and self-arranging
- ✓ another classification: Wolfram's or Langton's cellular automata

(*) from "Emergence", Stephen Johnson, Scribner

Common global properties of CS
"More is different", phase transitions

- ✓ Philip W. Anderson's 1972 "more is different" slogan:
  - criticism of the reductionist/constructionist hard line: "after discovering the fundamental laws, it is just a matter of reconstructing from them"
  - ...however, particle physics does not help solid state physics or biology!
  - reconstructionism crashes on the cliffs of *scale* and *complexity*
  - hierarchy levels of science show *qualitative* leaps (*new* properties)
  - psychology is not just applied biology, biology is not applied chemistry
  - [but this does not imply any unknown external force, either]
- ✓ notion of "critical mass"
  - ex: need enough ants for a pheromone trail to form
  - ex: need enough chemical types for an autocatalytic set to appear
- ✓ phase transitions in parameter space
  - broken symmetry
  - transition from randomness or chaos to order

Common global properties of CS
Decentralization & “more is different”?

✓ recap: decentralization (the “invisible hand”)

- no leader, no designer, no external organizing force that does not belong to the system
- the emergent properties entirely rely on the elements’ behavior and interactions among *themselves*

✓ recap: “more is different”

- ... but these properties cannot be *inferred* or *predicted* just by looking at the elements
- beyond a critical mass and across phase transition lines, the system exhibits *qualitatively new* behaviors

→ only an apparent paradox

- both aspects can, and actually *do* coexist in natural systems
- neither hard-line reductionism (“everything boils down to superstrings”)
- nor “vitalism” or intelligent design (“something else must be intervening”)

Common global properties of CS
Positive feedback

- ✓ positive feedback, circularity:
  - ex: ants bring more pheromone where there is pheromone
  - ex: termites bring pellets of soil where there is a heap of soil
  - ex: pigmented cells differentiate next to other pigmented cells
  - ex: fireflies want to synchronize with the swarm's flashes
  - ex: cars slow down where there are slow cars in front of them
  - ex: traders prefer buying stock that goes up
  - ex: the media talk about what is currently talked about in the media

→ amplification of fluctuations (nonlinearity)

→ instability of initially homogeneous state

→ broken symmetry

→ creation of structure

Computational Models of Complex Systems

Introductory Lecture 1

- Examples of complex systems 1
- Course organization
- Paper reviews (first period)

Introductory Lecture 2

- Examples of complex systems 2
- Common elementary features of CS
- Common global properties of CS