Lecture 1: What are Complex Systems?

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What are CS?

To provide a feeling for what complex systems are let us first remind ourselves on three other questions

- what is physics?
- what is biology and life sciences?
- what are social sciences?

By describing what these sciences are – and what they are not – we should develop a feeling of what complex systems are

The aim is to make clear that the science of CS is a derivative of the three disciplines and that this mix becomes something like a discipline by itself

Physics is the experimental, quantitative and predictive science of matter and its interactions

- quantitative statements are made: less ambiguous than words
- predictive means that statements are given in form of predictions which can be experimentally tested

Basically one asks specific questions to nature in form of experiments – and in fact, one gets answers. This methodology is unique in world history - the scientific method

What are CS?

What is physics?

Matter	**Interaction type**
Macroscopic matter	gravity, electromagnetism
Molecules	electromagnetism
Atoms	electromagnetism, weak force
Hadrons & leptons	electromagnetism, weak and strong force
Quarks & gauge bosons	electromagnetism, weak and strong force

All interactions in the physical world are mediated by the exchange of *gauge bosons*. For gravity the situation is not yet experimentally founded.

The nature of the fundamental forces

- Typically the four fundamental forces act homogeneously and isotropically in space (and time). There are famous exceptions however: the strong force or interaction acts in a way as if the interaction is limited to a 'string' – similar to type II superconductivity.
- These interactions work on different scales, from light years to femto meters: this means that one typically has to consider only one force for a given phenomenon of interest. The other one can be 100, 10^6, or up to 10^{39} times stronger than the other.
- Traditionally physics does not specify which particles interact with each other. Usually they all interact equally, the interaction strength depends on interaction type and the form of the potential.

What does predictive mean?

Assume you can do an experiment over and over again, e.g. drop a stone. The theoretical task is to predict the reproducible result.

Since Newton physics follows the following recipe

- Find the equations of motion to code your understanding of a dynamical system
$$\frac{dp}{dt} = F(x) \qquad , \qquad p = m\frac{dx}{dt}$$
- Predictive means: once F is specified the problem is solved, if the initial and or boundary conditions are known. The result is $x(t)$
- Compare the result with your experiments

Note: fixing initial conditions and boundary conditions means taking the system out of the context – out of the rest of the universe. This is why physics works!

The same philosophy holds for arbitrarily complicated systems. Assume a vector $X(t)$ represents the state of a system (for example all positions and momenta), then we get a set of equations of motion of this form

$$\frac{dX(t)}{dt} = G(X(t))$$

Predictive means that in principle you can solve these equations. However, these can be hard to solve.

Already for three bodies, this becomes an extremely hard task, the famous three-body problem (sun, earth, moon)

Laplace: if a daemon knowing all the initial conditions and able to solve all equations – we could predict everything

The problem is that this daemon is hard to find. In fact the Newton-Laplace program becomes completely useless for most systems. So are these systems not predictable?

What are CS?

What is physics?

Consider water and make the following experiment over and over again

- cool it to 0^{o}C – it freezes
- heat it to 100^{o}C – it boils almost certainly (under standard conditions)

One can maybe measure the velocity of a single gas molecule at a point in time, but not of all, $\mathcal{O}(10^{23})$ at the same time. But one can compute the probability that a gas molecule has a velocity v,

$$p(v) \propto \exp(-\frac{m}{2kT} v^2)$$

- For many non-interacting particles these probabilities become extremely precise and one can make predictions as before.
- Necessary: interactions are weak and the number of particles is large. Note that to compute the freezing temperature of water was impossible before simulations.

Note: The word prediction now has a much weaker meaning than in the Laplace-Newton sense. The concept of determinism is diluted.

What are CS?

What is physics?

The triumph of statistical mechanics

- The idea of statistical mechanics is to understand the macroscopic properties of a system from its microscopic components: relate the micro- with the macro world
- Typically in physics the macroscopic description is often simple and corresponds to the state of the phase in which the system is (solid, gaseous, liquid).
- Physical systems have often very few phases. A system is often prepared in one macro state (e.g. temperature and pressure is given). There are usually many possible microstates that are related to that macro state.
- In statistical mechanics the main task is to compute the probabilities for the many microstates that lead to that single macro state

Traditional physics works fine for a few particles (Newton-Laplace) and for many non-interacting particles (Boltzmann-Gibbs).

In other words, the class of systems that can be understood by physics is not so big.

There were more severe shifts to the concept of predictability

What does prediction mean? The crises of physics

Prediction in the 18th century is quite different from the concept of prediction in the 21st

- classical physics: exact prediction of trajectories

  →crisis 1900: too many particles →
- statistical physics: laws of probability allow stochastic predictions of the macro (collective) behavior of gases, assuming trajectories are predictable in principle

  →crisis 1920s: concept of determinism evaporates completely →
- QM and non-linear dynamics: unpredictable components – collective phenomena remain predictable

  →crisis 1990s: can not deal with strong interactions in stat. systems →
- Complex Systems: situation can be worse than QM: unpredictable components and complicated interactions – hope that collective is still predictable

What are CS?

What is physics?

What are complex systems from a physics point of view?

- many particle systems (as in statistical physics)
- may have stochastic components and elements (as e.g. in QM)
- interactions may be specific between two objects (networks)
- interactions may be of complicated type
- they are often chaotic (nonlinear equations of motion)
- interacting bodies are not limited to matter
- interactions are not limited to the 4 fundamental forces
- they can show very rich phase structure
- they can have many macro states, even simultaneously realized

Most physicists will not have a problem to call these extensions to traditional physics CS. For them it is still physics. The prototype model of CS in physics are the so-called *spin glasses*.

What are CS?

What is physics?

This is not yet what we believe what Complex Systems are – there are crucial concepts missing

- However, due to more specific interactions and the increased variety of types of interactions, the variety of macroscopic states changes drastically. These emerge from the properties of the system's components and the interactions. The phenomenon that a priori unexpected properties may arise as a consequence of the generalized interactions is sometimes called emergence. Such CSs can have an extremely rich phase structure.
- In the case when there is a plurality of macro-states in a system, this leads to entirely new questions one can ask to the system:
  - What is the number of macro states?
  - What are their co-occurrence rates?
  - What are the typical sequences of occurrence?
  - What is their life-times?
  - What are the transition probabilities? etc.

What are CS?

What is physics?

What we definitely want to keep from physics

CS is the experimental, quantitative and predictive science of generalized bodies with generalized interactions

Generalized interactions are described by the interaction type, and who interacts with whom. If there are more than 2 objects involved, interactions are conveniently indicated by networks

$$A_{ij}$$

Interactions themselves remain based on concept of exchange. For example think of communication, where messages are exchanged, trade where goods and services are exchanged, friendships where wine bottles are exchanged, etc.

For many CS the framework of physics is incomplete: What are the missing concepts? non-Equilibrium, co-evolution, adjacent possible, ...

A note on chemistry – the science of equilibria

- In chemistry interactions between atoms and molecules can be already quite specific. So why is chemistry usually not a CS?
- Classically, chemistry is based on the law of mass action – many particles interact in a way to reach equilibrium.

$$\alpha A + \beta B \rightleftharpoons \sigma S + \tau T$$

$\alpha, \beta, \sigma, \tau$ are the stoichiometric constants, k_+, k_- are reaction rates
forward reaction: $k_+ A^\alpha B^\beta$
backward reaction: $k_- S^\sigma T^\tau$

they are the same in equilibrium

$$K = \frac{k_+}{k_-} = \frac{\{S\}^\sigma \{T\}^\tau}{\{A\}^\alpha \{B\}^\beta}$$

What are CS?

A note on chemistry

- Many CS are characterized by the fact that they are out of equilibrium. This means that there are no fixed point type equations that can be used to solve the problem.
- In this situation the help from statistical mechanics becomes very limited. It is extremely hard to handle systems which are out of equilibrium.
- Even the so-called stationary non-equilibrium is extremely hard to understand – even computationally (thermostats)
- On the positive side: many CS are self-organized critical

let's keep from chemistry

> Many CS are out of equilibrium
> Many CS are non-ergodic

Note: as soon as one focuses on e.g. cyclical catalytic reactions on networks chemistry becomes a CS very soon

What are CS ?

What is biology?

Life Science is the experimental science of living matter.

What is living matter?

What are the minimal conditions for living matter to exist?
According to S.A. Kauffman

- living matter has to be self-replicating
- has to run through at least one Carnot cycle

What are CS?

What is Biology?

- Living matter is a self-sustained sequence of genetic activity over life.
- It uses energy and performs work. It is constantly out of equilibrium.
- Genetic activity has to do with chemical reactions which take place e.g. within cells (compartments). Unfortunately, this is only partly true. Chemical reactions usually involve billions of atoms or molecules.
- What happens in the cell is chemistry with few molecules. If you have a few molecules only, there arise problems:
  - the law of large numbers becomes inappropriate
  - the laws of diffusion become inadequate
  - the concept of equilibrium becomes shaky
  - without equilibrium what is the law of mass action?
- If we do not have a law of mass action, how is chemistry to be done?

Consequently, traditional chemistry is inadequate for living matter

More complications in the cell:

- Molecules may be transported from site of production to where they are needed. This changes law of diffusion even more, it becomes anomalous diffusion, $\frac{d}{dt}p(x,t) = D\frac{d^{2+\nu}}{dx^{2+\nu}}p(x,t)^{\mu}$.
- Chemical binding depends on 3D structure of molecules.
- Chemical binding depends on 'state' of molecules, e.g. if they are phosphorylated or not.
- 'Reaction rates' – if one still wants to use this term – depend on the statistical mechanics of small systems, i.e. fluctuation theorems might become important.

Biological interactions happen on networks – almost exclusively

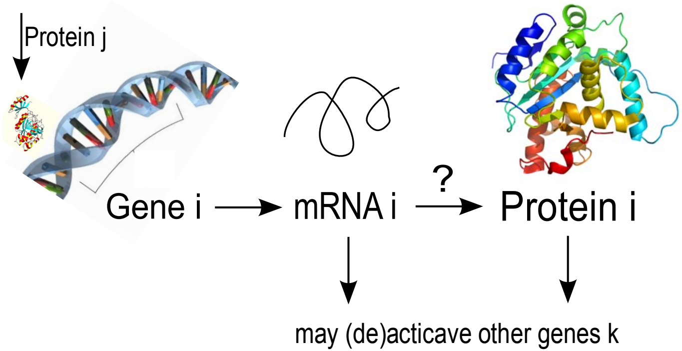
- Genetic regulation governs the temporal sequence of abundance of proteins, nucleic material and metabolites within a living organism
- Genetic regulation can be viewed as a discrete interaction
- Protein-protein binding is discrete, for example complex formation

Discrete interactions are described by networks:

- gene-regulatory network (e.g. Boolean)
- metabolic network
- protein-protein network

What are CS?

What is Biology?



Nothing in biology makes sense except in the light of evolution. Dobzhansky

Genetic material and the process of replication involve several stochastic components, and lead to variations in copies. Replication and variation are two of the three main ingredients for all evolutionary processes.

What is evolution? Remember the Darwinian story

Consider a population of some kind. The offspring of this population has some random variations (e.g. mutations). Individuals with the optimal variations (given a certain surrounding) have a selection advantage, i.e. fitness. This fitness manifests itself such that these individuals have the more offspring, and thus pass on the particular variation on to a new generation. In this way 'optimal' variations get selected over time.

Is this definition predictive science? Or is it just a convincing story?
Is the Darwinian story falsifiable? How can we measure fitness? It is an *a posteriori* concept. Survival of the fittest $\equiv$ survival of those who survive.

Evolution is a three-step process.

1. new thing comes into being in a given environment.
2. new thing has the chance to interact with environment. The result of this interaction: possibility to get selected or destroyed.
3. if the new thing gets selected (survives) in this environment it becomes part of this environment – it becomes part of the new environment for all future, new and arriving things.

Evolution happens simultaneously on various scales (time & space): cells – organisms – populations

Evolution is not physics.

If you think of this three step process in terms of equations of motion

1. Write down the dynamics of the system in the form of equations of motion.
2. Boundary conditions depend on these equations – you can not fix them.
3. Consequently, you can not solve the equations.
4. Newtonian recipe breaks down, you fail – program becomes mathematical monster if you think of dynamically coupled boundary conditions with the dynamical system.

The task is: try to solve it nevertheless. We will see that multi-scale methods can be used to address this type of problems.

The concept of evolution is fundamentally different from physics.

It is immediately evident that we are confronted with two huge problems:

- Boundary conditions can not be fixed.
- Phase space is not well defined – it changes over time. New elements may emerge that change the environment substantially.

The evolutionary aspect is essential for many CS, it can not be neglected.

Finding a language for evolutionary processes – the adjacent possible

This 'science' is at its very beginning. Maybe not even the right language has been established so far.

- The adjacent possible is the set of all possible worlds that could potentially exist in the next timestep. The adjacent possible depends strongly on the present state of the world.
- With this definition evolution is a process that continuously fills the AP.
- Different from physics: a given state determines the next state. In physics all potential states are known.
- Evolution: given state determines the realization of a (huge) set of possible states. The future states may not even be known at all – 'creative process'.
- The filling of the adjacent possible determines the next adjacent possible.

We have learned for evolutionary processes

- One can not fix boundary conditions of evolutionary systems. This means that it is impossible to take the system apart without possibly losing critical properties. Here the triumphal concept of reductionism starts to become inadequate.
- Evolutionary CS feel their boundary conditions.
- Evolutionary CS change their boundary conditions.
- In physics the adjacent possible is very small. For example imagine a falling stone. The AP is that it is on the floor in two seconds. There are practically no other options.
- Lagrangian trajectories are completely specified by initial & end point. In evolution the AP evolves: $\mathrm{AP}(t) \rightarrow \mathrm{AP}(t+1) \rightarrow \mathrm{AP}(t+2) + \cdots$
- In physics the realization of the AP does (almost) not influence the next AP.

Biological systems are adaptive and robust – the concept of the edge of chaos

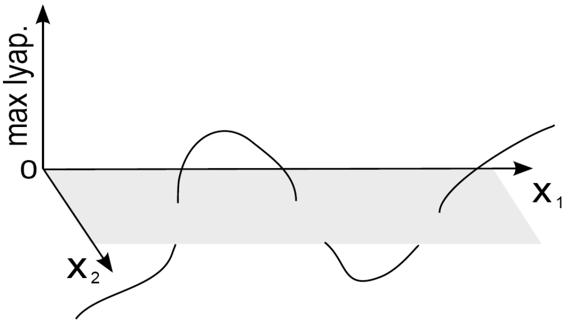
The possibility to adapt and robustness seem to exclude each other. However, living systems are clearly adaptive and robust at the same time. To explain how this is possible one can take the picturesque view:

- Every dynamical system has a maximal Lyapunov exponent. It measures how – two initially infinitesimally close trajectories – diverge over time. The exponential rate of divergence is the Lyapunov exponent λ,

  $$|\delta X(t)| \propto e^{\lambda t}|\delta X(0)|$$

  where $\delta X(0)$ is the initial separation
- If the exponent is positive the system is called chaotic, or strongly mixing
- If the exponent λ is negative the system approaches an attractor – two initially infinitesimally adjacent trajectories converge. The system is periodic
- If the exponent is zero: the system is called quasi-periodic, or 'at the edge of chaos'.

How does nature find the edge of chaos?



The set of points where the Lyapunov exponents are zero is usually of measure zero. However, evolution seems to find and select these points.

How does nature find the edge of chaos?

How can a mechanism of evolution detect something of measure zero?

- One explanation is self-organized criticality, where systems organize themselves to operate at a critical point between order and randomness. SOC can emerge from interactions in different systems, including sand piles, precipitation, heartbeat, avalanches, forest fires, earthquakes, etc.
- Or is this set simply not of measure zero?

Biological systems are self-organized and critical

- Self-organized systems are dynamical systems that have a critical point as an attractor. Very often these systems – at a macroscopic scale – are characterized by scale invariance. Scale invariance means the absence of a characteristic (length) scale.
- A critical point of a system is reached at conditions (temperature, pressure, slope in sandpile, etc.) where the characteristic length-scale (e.g. correlation length) becomes divergent.

Applications cover all the sciences
Physics: particle-, geo-, plasma-, solar physics, cosmology, quantum gravity,...
Biology: evolutionary biology, ecology, neurobiology, ...
Social sciences: economics, sociology, ...

What are CS?

What is Biology?

An intuition for self-organized critical systems – sandpile models

Imagine a pile of sand.

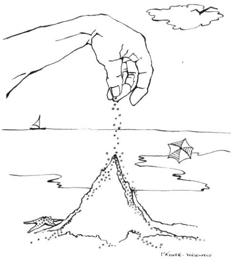


Fig. by Wiesenfeld

- If the slope is too steep avalanches go off → slope becomes flatter
- If the slope is too flat sand gets deposited → slope becomes steeper

The pile self-organizes toward a critical slope. The system is robust and adaptive.

Let us collect the components for CS that we get from the life sciences

- Interactions take place on networks
- Out of equilibrium
- Evolutionary dynamics
- Core components are discrete – e.g. Boolean networks
- Adaptive and robust: edge of chaos – self-organized critical
- Memory: processes have memory (non-Markovian)

What are CS ?

What are CS?
What is social science?

Social science is the science of social interactions and their implications to society.

Traditionally it is neither quantitative nor predictive, nor does not produce experimentally testable predictions. Why is that so?

- Lack of detailed data
- Lack of reproducibility / repeatability

The queen of the social sciences is economics, i.e. the science of the invention, production, distribution, consumption, and disposal of goods and services.

All of these components happen on networks, i.e. the associated interactions are very much directed and interconnected. Maybe network aspects are most illustrative when studied in the social sciences, even more than in the life sciences.

What are CS?

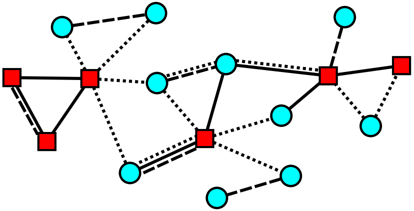
What is social science?

What are societies?

- People, goods or institutions are represented by nodes of a network.
- Interactions are represented by links in networks of various types.
- One node may be engaged in several types of interaction.
- Nodes are characterized by 'states': wealth, opinion, age, etc.
- Nodes and links change over time.

What are societies?

- Societies are co-evolving multiplex networks, $M_{ij}^{\alpha}(t)$
- A multiplex network is a collection of networks on the same set of nodes



Links. $\alpha = 1$: communication: full line; $\alpha = 2$: trading: dashed line; $\alpha = 3$: friendship: dotted line.

States. blue – votes for Tsipras; red – votes for Merkel.

- Nodes i (humans or institutions) are characterized by states, or state vectors, $\sigma_i(t)$

Let us collect the components for CS that we get from the social sciences

- Interactions happen on a collection of networks (Multiplex networks).
- Networks may interact with themselves.
- Networks show a rich variety in growth and re-structuring.
- Networks are evolutionary and co-evolutionary objects.

What are CS?

What is co-evolution?

The concept of co-evolution.

- What is an interaction? In general an interaction can change the state of the interacting objects, or the environment. For example, the collision of two particles changes their momentum. The magnetic interaction of two spins may change their orientations. An economic interaction changes the portfolios of the participants involved.
- The interaction partners (network or multiplex) of a node can be seen as the 'environment' (space) of that node. The environment determines the future state of the node.
- Interactions can change over time. For example people establish new friendships or economical links, countries terminate diplomatic relations. The state of nodes determine the future state of the link, meaning if it exists in the future or not.

The state (topology) of the network determines the future states of the nodes. The state of the nodes determines the future state of the links of the network.

What are CS?

A pictorial view

Co-evolving multiplex networks – more formally.

$$\frac{d}{dt}\sigma_i^{\alpha}(t) \sim F\left(M_{ij}^{\alpha}(t), \sigma_j^{\beta}(t)\right)$$

and

$$\frac{d}{dt}M_{ij}^{\alpha}(t) \sim G\left(M_{ij}^{\alpha}(t), \sigma_j^{\beta}(t)\right)$$

This is maybe the simplest way to illustrate what a CS is, or looks like.

- Networks are observable (big data)
- Collections of networks are manageable
- States of individual nodes are (will be) observable

From a practical point of view it is useless, because *G* and *F* are not specified. They can be stochastic. However, it should be possible to express most CS of the form we discussed in this form.

What are CS?

What are CS – a summary.

CS as we understand them today emerged from physical sciences, life sciences and the social sciences.

- Interactions happen on (dynamical) networks or multiplex NWs
- Interactions involve all sorts of objects (nodes) and interaction types (links)
- System influences and feels its boundary
- Dynamics is non-linear (no possibility for superposition principle)
- Dynamics is evolutionary ('creative', robust, adaptive, phase space not fixed)
- States of system and the interactions are co-evolving
- They are non-ergodic, non-Markovian
- Description must be quantitative, predictive and experimentally testable

What are CS?

Some famous triumphs of science of CS.

- Network theory
- Genetic regulatory networks
- Genetic algorithms
- The Santa Fe stock market
- Theory of decreasing returns
- Origin and development of languages
- Mosaic vaccines
- Models in epidemiology
- Understanding of systemic risk in financial markets
- Scaling in biology and urbanization