Introduction

Computational Models for Complex Systems

Paolo Milazzo

Dipartimento di Informatica, Università di Pisa
http://pages.di.unipi.it/milazzo
milazzo@di.unipi.it

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About this course

General info:

- Course web page
  `http://pages.di.unipi.it/milazzo/teaching/AA1920-CMCS/`
- Teaching hours (Aula Fib L1)
  - Wed 9-11
  - Fri 16-18
- Office hours
  - should be Tue 15-17, but
  - better if we fix an appointment via email...

About this course

Teaching info:

- Contents of this course
  - Methods for the modeling, simulation and formal analysis of complex systems such as populations, biological systems, social networks, markets, etc...
- Textbooks and software
  - No unique textbook and software tool.
  - A number of lecture notes and references to useful software tools will be made available on the course web page.
  - Also the slides of the course will be made availble on the web page
- Exam
  - It may consist in either a presentation of a scientific paper, a small project (to be done in groups of 1-3 students), or a standard oral exam.
  - Proposals of scientific papers and projects ideas will be made available close to the end of the course (proposals from students are welcome!)
  - If possibile, a first round of student presentations will be organized before the end of the course (last couple of lessons)

Computational Models for Complex Systems

Computational models? Complex systems?

WHAT ARE WE TALKING ABOUT??

Let's start from understanding what, in general, is a

MODEL of a SYSTEM

Understanding requires modeling

Assume we want to

- understand how a given system works
- or that we want to design a new system.

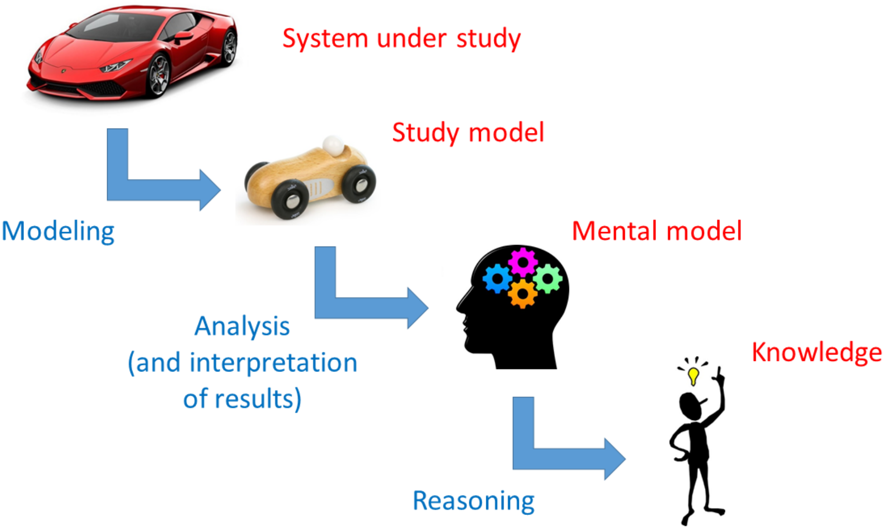
First of all, we need to build a model!

$\Rightarrow$

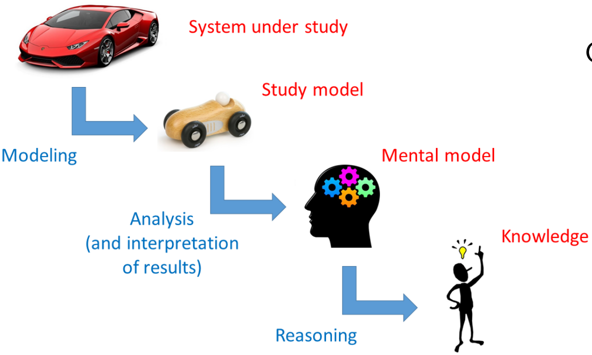
Definition: Model

A model is a simplified and approximate representation of a system, that allows reasoning on the system's properties

Understanding requires modeling



Sources of error



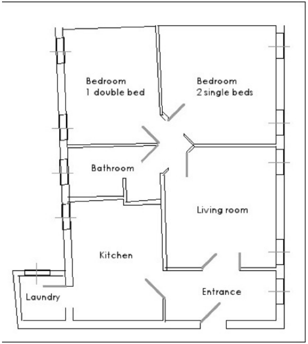
Common sources of error:

- Model inaccuracy
- Analysis method inaccuracy
- Analysis results ambiguity
- Inaccurate reasoning

Inaccuracies and ambiguities can be limited by adopting well-established scientific methods and rigorous (logical) reasoning techniques

Examples of models

From Architecture:



Planimetries/projects

Scale models

These are models of artificial entities (buildings) useful to assess structural properties at design time, and to let the buyer evaluate the result in advance

Examples of models

From Architecture:

Renderings

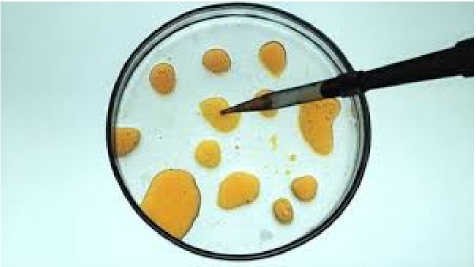
Virtual Reality

Computer-based techniques are nowadays more accurate and realistic than traditional approaches, and offer advanced interaction possibilities

Examples of models

From Life Sciences:

In vivo models
(mice, rats, pigs, ...)

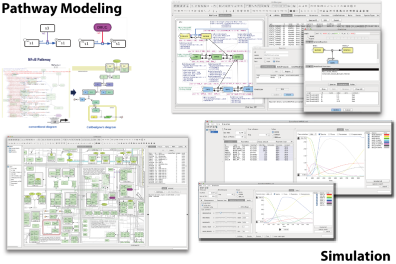


In vitro models
(cells in a test tube or Petri dish)

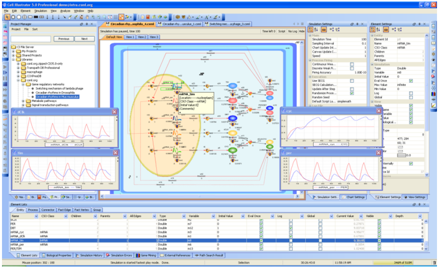
These are models of the human being, typically used to create new knowledge (on diseases, toxicity effects, etc...)

Examples of models

From Life Sciences:



In silico models



In silico models

Computer-based techniques are usually faster and cheaper than *in vivo* and *in vitro* methods, and sometimes they have comparable accuracy.

Mathematical modeling

Mathematics provides tools for building abstract models of almost everything

- geometry for Architecture
- differential equations for Weather

Properties of mathematical models (corresponding to properties of the modeled system) can be studied either

- analytically
  (e.g. the volume of a building, or the payload of a bridge, can be computed precisely)
- or numerically
  (e.g. weather forecasts, are based on approximate simulations)

Numerical analysis of mathematical models is quite similar to computational modeling

Computational modeling

Definition: Computational Model

A computational model is a mathematical representation of a dynamical system taking a computer-executable form.

First of all, with this definition we are restricting the class of systems of interest to dynamical systems (systems which evolve over time).

- So, e.g. the computer-based architectural models are not computational models, since building are not dynamical systems.

Then, a mathematical representation is necessary, since mathematics provides unambiguous (formal) tools to represent systems.

- An ambiguous model could be interpreded differently by the modeler and the computer

Computer-executable means that the computer should be able to compute the evolution of the system over time (e.g. by performing simulations)

Focus on dynamical systems

Dynamical systems are systems that evolve by changing their state over time

The state of a dynamical system is usually represented by a finite set of variables called state variables

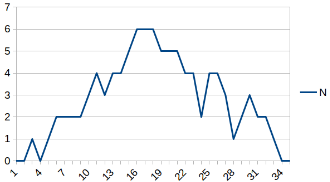
- temperature, humidity, price, position, ...

The state of the system (i.e. the values of the variables) can change in either a discrete or a continuous way (or both)

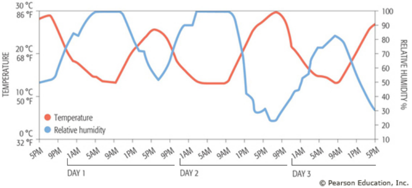
Focus on dynamical systems

Some simple examples:

- Queue at the post office.
  State variable: N (number of enqueued people)

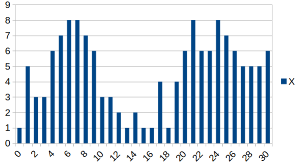
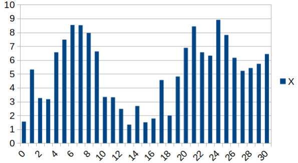
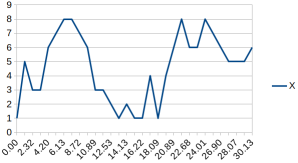
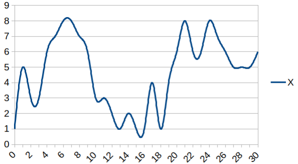


- Weather.
  State variables: T (temperature), H (humidity)



Focus on dynamical systems

Dynamical system span over a discrete/continuous spectrum

<table>
<tr><th></th><th>Discrete States</th><th>Continuous States</th></tr>
<tr><th>Discrete Time</th><td>State variables in $\mathbb{N}$ (or $\mathbb{Z}$)
time variable t in $\mathbb{N}$

</td><td>State variables in $\mathbb{R}_{\geq 0}$ (or $\mathbb{R}$)
time variable t in $\mathbb{N}$

</td></tr>
<tr><th>Continuous Time</th><td>State variables in $\mathbb{N}$ (or $\mathbb{Z}$)
time variable t in $\mathbb{R}_{\geq 0}$

</td><td>State variables in $\mathbb{R}_{\geq 0}$ (or $\mathbb{R}$)
time variable t in $\mathbb{R}_{\geq 0}$

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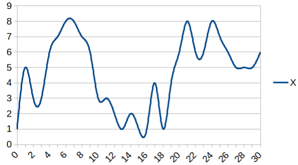
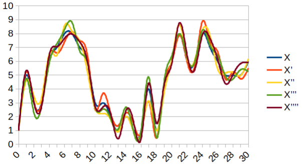
Focus on dynamical systems

Moreover, dynamical systems (and/or their models) can be deterministic or probabilistic/stochastic

<table>
<tr><th>Deterministic</th><th>Stochastic</th></tr>
<tr><td>Unique dynamics
for each initial state</td><td>Different dynamics
from the same initial state</td></tr>
<tr><td>
</td><td>
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Different types of systems should be modeled with different types of models

- Otherwise, approximations come into play

Why should we model dynamical systems?

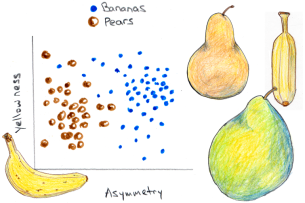
Models of dynamical systems can be used to study (on a computer)

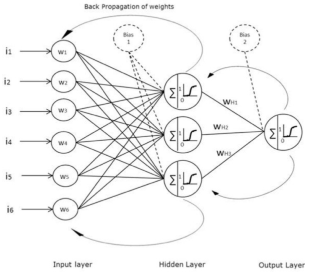
- Reachability of states (predictions)
  - Will it rain tomorrow?
  - Will this drug cause toxicity?
  - Will vaccinations eradicate the disease?
  - Will this content spread in a social network?
- Behavioral patterns
  - Will the concentration of this substance become stable?
  - Will the size of the population oscillate?
  - Will cars stay out of the city center?
- Effects of perturbations/control strategies
  - What happens to the disease if we change the dosage of a drug?
  - What happens to fish populations if we stop fishing for one month?
  - Which impact would have the closure of a street?

How to build a computational model?

The Data-driven way (e.g. Machine Learning)

- The model is directly inferred from data
- Usually requires a lot of data, but limited knowledge about the system functioning
- The model takes a form suitable for inference method used (e.g. a Neural Network)
- If enough data is available, it often works very well (good predictions)
- Inferred models are often very difficult to be interpreted





How to build a computational model?

The Knowledge-driven way (e.g. this course!)

- The model is constructed on the basis of the available knowledge about the system's internal mechanisms
- Usually requires limited data, but a good knowledge about the system functioning
- The model takes a form suitable to describe the system's internal mechanisms
- Model construction usually requires some effort, and ofter predictions suffer from approximations, but
  - the method works also when few data are available
  - the model is interpretable: it contributes to understending why a system behaves as observed
  - modeling allows validating hypotheses on the system functioning

Complex systems

Putting the pieces together, we have more or less understood what is a

COMPUTATIONAL MODEL of a DYNAMICAL SYSTEM

but this course deals with COMPLEX systems... what do they are?

Complex systems a particular class of dynamical systems...

Complex systems

Definition: Complex system

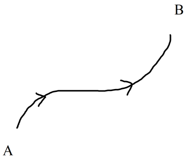
A complex system is a system consisting of many simple components interacting with each other, from whom a collective behavior with interesting dynamical properties emerges.

Complex system's behavior out of simple component interactions

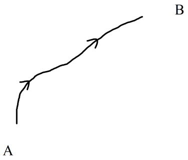
- Holistic interpretation: "the whole is more than the sum of the parts"
- The behavior of the system emerges, it is not easily predictable from the knowledge of the individual components

Examples of complex systems

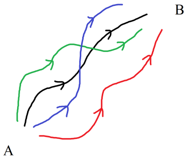
Flocking of birds



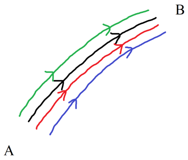
One bird



Another bird



Four separate birds



Four birds in a flock

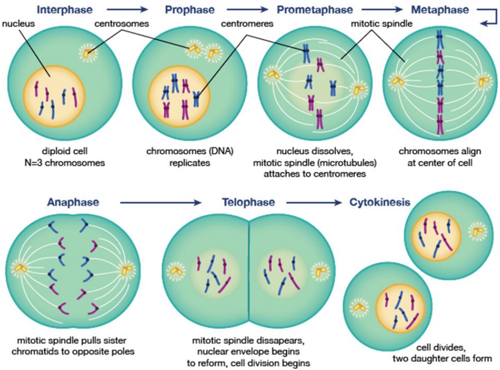
Examples of complex systems

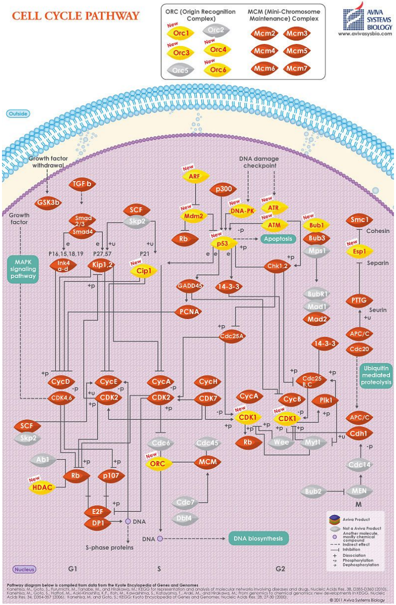
In the flocking example:

- the complex system is the flock
- the simple components are the birds
- the individual behavior of each component is "fly towards destination"
- the interactive behavior of each component is "fly close to the other birds, follow the leader"
- the emergent behavior (of the flock) is "maintain the typical V-shape"

Examples of complex systems

The cell cycle
(process leading to cell duplication)





Examples of complex systems

In the cell cycle example:

- the complex system is the cell
- the simple components are the biomolecules (DNA, proteins, etc...)
- the individual behavior of each component is
  "be sinthesized and degraded"
- the interactive behavior of each component is
  "participate in chemical reactions"
- the emergent behavior (of the cell) is
  "growth and division into two cells"

Examples of complex systems

Ants foraging (search for food)

When a colony of ants finds a source of food, they organize in a trail along the path from their nest to the food source

This is obtained through a mechanism called stigmergy

- indirect coordination mechanism: ants leave drops of a chemical along the path, other ants follow such a trace and reinforce it by leaving additional drops

Examples of complex systems

In the ants foraging example:

- the complex system is the ant colony
- the simple components are the ants
- the individual behavior of each component is "go around, looking for food"
- the interactive behavior of each component is "leave, detect and follow drops of chemicals"
- the emergent behavior (of the colony) is "trail formation"

Differently from the birds and biomolecules in the previous examples, ants commmunication is not direct, but mediated by the environment (where drops are left)

Examples of complex systems

Traffic

Examples of complex systems

In the traffic example:

- the complex system is the urban mobility system
- the simple components are the cars
- the individual behavior of each component is
  "drive to destination, according to the rules"
- the interactive behavior of each component is
  "avoid crashes"
- the emergent behavior (of the colony) is
  "queues"

Again, the environment plays a role. Streets are a limited resource that is shared by cars

- when the number of cars exceeds the street capacity, queues start to form

Examples of complex systems

Social networks

Examples of complex systems

In the social network example:

- the complex system is the network
- the simple components are the members (profiles)
- the individual behavior of each component is "expose your profile"
- the interactive behavior of each component is "share and look at other's shares, communicate"
- the emergent behavior (of the network) is "trend topics, formation of communities, ..."

These networks are dynamic

- their strucure (connections) evolve over time
- network science is the discipline that studies the evolution of network structures
- in complex networks, interesting global topologies emerge from local changes (like in complex systems)

Modeling notations for complex systems

Many modeling languages are available for complex systems

From mathematics:

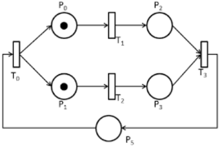
- Recurrence relations
- Differential equations

$$X_t = 2X_{t-1}Y_{t-1} - 3$$

$$\dot{X} = 2XY - 3$$

From concurrency theory:

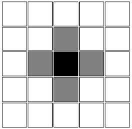
- Petri nets
- Multiset rewriting
- Process calculi



$$A + B \to C \qquad a.P \mid \overline{a}.Q$$

From artificial life:

- Cellular automata
- Agents



```
to eat-grass
  ask turtles [
    if pcolor = green [
      set pcolor black
      set energy energy + 10
    ]
  ]
end
```

From modeling notations to behaviors

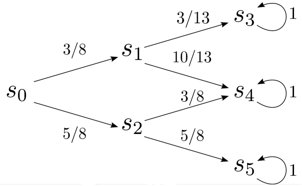
Modeling languages allow the modeler to express

- the relationships between the state variables of the system,
- and the rules/laws that determine the change of their values over time

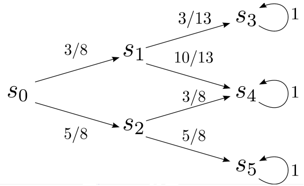
The dynamics (or behavior) of the system (the actual sequences of states reached by the system over time) can be computed according to the semantics of the modeling language

- Semantics gives a meaning to a language

The semantics of a modeling language can often be expressed as a transition system



Analysis of behaviors



Once you a have a descrition of the system's behavior (the transition system) you can analyze it in several ways:

- simulation (computes a trace of the transition system)
- model checking (determine whether the whole transition system satisfies a given dynamical property)
- ... static analysis, steady state analysis, sensitivity analysis, ...

Simulation does not require constructing the whole transition system

Modeling vs programming

Modeling and programming are very similar

- a program is somehow a model of a function

dynamical system		function
$\Downarrow$	syntax	$\Downarrow$
model (in a suitable language)		program (in a suitable language)
$\Downarrow$	semantics	$\Downarrow$
dynamics		meaning
$\Downarrow$	analysis	$\Downarrow$
simulation model checking		testing model checking ....

Workplan

This is the (tentative) schedule of this course:

- Mathematical modeling of dynamical systems
  - Discrete models (recurrence equations)
  - Continuous models (ordinary differential equations - ODEs)
- The chemical reaction metaphor
  - From ODEs to stochastic simulation
- Transition systems and model checking
- Modeling notations:
  - Multiset rewriting
  - Petri nets
- Discrete event simulation
- Structured approaches:
  - Agent-based modeling and simulation
  - Interactions over a network

Workplan

We will see applications to:

- social behaviors of animals (e.g. prey-predator interaction, flocking)
- epidemiology (e.g. spread of diseases and vaccination)
- biology (e.g. cell pathways)
- social systems
- manufacturing
- ...

Software

Software we will use:

- your favorite spreadsheet (Excel, Openoffice calc, Google docs, ...)
- GNU Octave (`https://www.gnu.org/software/octave/`)
- Dizzy stochastic simulator (available on the course web page)
- PRISM Model Checker (`https://www.prismmodelchecker.org/`)
- NetLogo (`https://ccl.northwestern.edu/netlogo/`)
- Java (or any other programming language...)