OUTLINE

INTRODUCTION BY EXAMPLES

COURSE TOPICS: AN OVERVIEW

Modelling: An introduction

A MOTIVATIONAL GLANCE

Science is the driver of our times.

Stephen Emmott Chief of Computational Sciences Microsoft Research Cambridge

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Facing these challenges passes through our ability to understand their functioning and control their behaviour.

This is the major scientific challenge of the 21st Century!

Computational Science is the driver of our times.

Paraphrasing Stephen Emmott :-)

A MOTIVATIONAL GLANCE

Computational Science is the driver of our times.

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The level of complexity, the size of those systems, the large amount of experimental data, require vast computational power to be processes.

And clever mathematics and algorithms to do it!! Beyond the current state of the art...

WHAT IS A COMPLEX SYSTEM?

FROM WIKIPEDIA

A complex system is a system composed of interconnected parts that as a whole exhibit one or more properties (behavior among the possible properties) not obvious from the properties of the individual parts.

The original Latin word complexus signifies entwined or twisted together (Heylighen, 1996).

EXAMPLES OF COMPLEX SYSTEMS

Complex systems are ubiquitous in the world.

- Biological systems
- Ecological systems
- Physical systems
- Computer systems
- Socio-economical systems
- ...

COMPLEXITY

Complexity can be defined as "the name given to the emerging field of research that explores systems in which a great many independent agents are interacting with each other in many ways" [Waldrop, 1992]

[Complexity is] "that property of a language expression which makes it difficult to formulate its overall behaviour, even when given almost complete information about its atomic components and their interrelations." (Edmonds, 1999)

from R. Frei, G. Di Marzo Serugendo: Concepts in complexity engineering. IJBIC 3(2): 123-139 (2011).

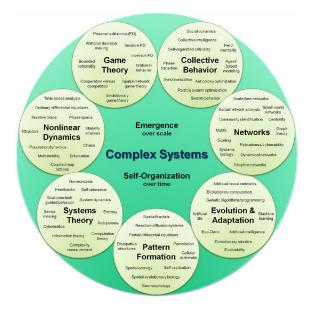
COMPLEXITY

Complexity is characterised by non-linear relationships between parts, openness, feedback loops, emergence, pattern formation, and self-organisation (Grobbelaar and Ulieru, 2007).

NON-LINEARITY

In linear systems, effect is directly proportional to cause, whereas in non-linear systems, the effect may be any. Non-linearity comes in many flavours, tending to occur when a system's interactions are multiple, ecologically embedded, non-additive, inseparable, heterogeneous, interactive, asynchronous, lagged, or delayed (Bullock and Cliff, 2004).

FEATURES OF A COMPLEX SYSTEM



EMERGENT BEHAVIOURS

Emergence describes how order appears out of chaos (Holland, 1998).

Most systems which exhibit emergence can be modelled in terms of the interaction of agents. Building blocks are combined to form a higher level system. Emergent phenomena are often hierarchical: complex ones are composed of simpler ones (Holland, 1995).

EMERGENT BEHAVIOURS

Emergence is a bottom-up effect, which generates order from randomness (Mueller-Schloer, 2004).

It results in a self-organised increase of order, in space or time. A global behaviour arises from the interactions of its local parts; cannot be traced back to the individual parts (De Wolf and Holvoet, 2005).

None of the entities composing the system knows how to achieve the emergent phenomenon (Di Marzo Serugendo et al., 2006b).

AN EXAMPLE: EL BOTTELLÓN.

El bottellòn refers to a phenomenon in the city of Granada, Spain: people in the nights spontaneously gather in a square in the city and start a big drinking party.





ADAPTIVITY AND SELF-ORGANIZATION

"Self-organisation is the dynamical and adaptive mechanism or process enabling a system to acquire, maintain and change its organisation without explicit external command during its execution time; there is no centralised or hierarchical control. It is essentially a spontaneous, dynamical (re-) organisation of the system structure or composition."

Adaptation means achieving a fit between system and environment; thus, every self-organising system adapts to its environment (Heylighen, 2003).

ADAPTIVITY AND SELF-ORGANIZATION

Self-organization is strongly related to the concept of emergence.

It usually refers to systems that are made up of atomic components that have a form of "intelligence" (i.e. small robots, bird flocks, schools of fishes).



AN HIGH LEVEL VIEW ON CS

HIGH LEVEL VIEW

We will look at complex systems made up of entities interacting in complex ways (population models).

ENTITIES?

Entities can be of different nature: molecules, cells, animals, computer jobs, processors, humans, ...

INTERACTIONS?

Interactions can involve a small or large number of entities, and may depend in complex ways from the environment or the global state of the system (non-linearity)

FEATURES

Non-linearity, emergent behaviour, self-organization, adaptivity, openness, robustness, evolutionary aspects,

MODELLING COMPLEX SYSTEMS

Essentially, all models are wrong, but some are useful.

George E. P. Box

WHAT IS MODELLING?

Modelling means constructing a formal object, based on some mathematics, which is an abstract representation of the reality. As such, any model is wrong. But we hope it to be sufficient to capture some aspects of the phenomenon studied. Any model of complex systems requires experimental data to be tuned and validated.

MODELLING COMPLEX SYSTEMS

THE GOALS OF MODELLING

Modelling has two main goals: explanation and prediction.

EXPLANATION: identify the key ingredients that drive the observed behaviour of the phenomenon of interest.

Prediction: predict the behaviour of the system under different situations.

These two goals are somehow in conflict for complex systems: explanation calls for abstraction, prediction for detail.

QUALITATIVE VERSUS QUANTITATIVE

Models can be qualitative, essentially capturing possible behaviours, but without giving "numbers", or quantitative, giving quantitative predictions of measurable quantities (when and if measurement is possible).

MODELLING COMPLEX SYSTEMS

MATHS FOR QUANTITATIVE MODELS

We will be interested in the temporal behaviour of systems.

We will consider some key ingredients for the maths:

ENTITIES: can be modelled as discrete objects or continuous

quantities.

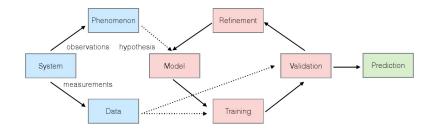
EVOLUTION: can be (non)-deterministic or stochastic.

TIME: can be discrete or continuous.

By choosing a combination of the ingredients above, we obtain different mathematical objects to work with:

- Discrete or continuous time Dynamical systems (DTDS, ODE, PDE, SDE);
- Stochastic Processes (discrete or continuous time Markov Chains)
- Hybrid systems (a mixture of the above)

MODELLING CYCLE



IMPORTANT ISSUES

- VALIDATION Model has to be fitted to experimental data and then validated in its explicative/predictive power.
- DATA PROBLEM Technological improvements permit the generation of huge amount of data. One needs to make sense of them.
- COMPUTATIONAL PROBLEM Model simulation and analysis can be extremely costly from a computational viewpoint (large models), but also model fitting and data analysis.