Computational Modelling
Introduction

Luca Bortolussi[1]

[1]Department of Mathematics and Geosciences
University of Trieste

Office 328, third floor, H2bis
luca@dmi.units.it

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Course organisation

Lectures and lab

- "Standard" lectures introducing basic concepts and techniques
- Computational Lab: implementation
- Modelling lab: model analysis
- "Non-standard" lectures (?): paper discussions, paper reading in group.

Exam

- Seminar on a project work: Modelling and analysis of a system (to be chosen).

Timetable

- 72 hours course!!! Better if we do 7 hours per week....

Outline

A MOTIVATIONAL QUOTE

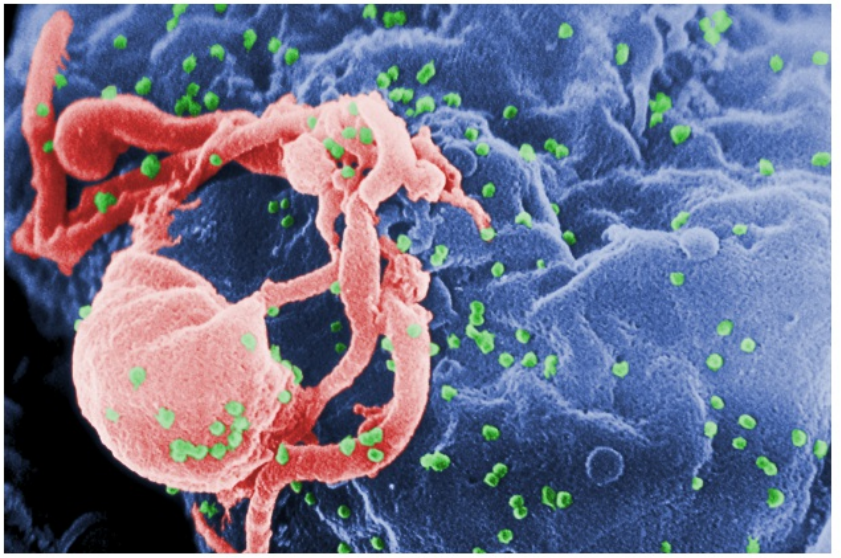
Science is *the* driver of our times.

Stephen Emmott
Chief of Computational Sciences
Microsoft Research Cambridge

Data Centre efficiency

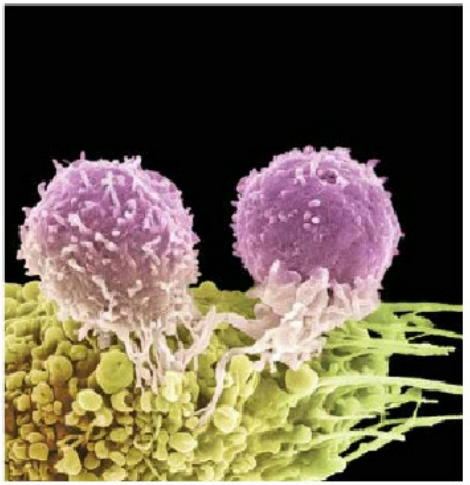
- We want to reply to all customer requests with small latency.
- We want to consume as few energy as possible.
- There is a trade off between these two goals. How many servers do we need for a good compromise?

HIV DRUG DOSAGE



- HIV therapies require the assumption of drug cocktails for long periods of time.
- How do we find the best cocktail for a given patient?
- And how do we plan the drug dosage for it to be the most effective for a given patient?

CANCER AND THE IMPORTANCE OF NETWORKS



T lymphocytes and cancer cell

Coloured scanning electron micrograph (SEM) of two T lymphocyte cells attached to a cancer

WHAT IS CANCER?

- Is Cancer a disease of genes?
- Is Cancer a disease of biological pathways?
- Is Cancer a disease of interaction networks?
- Is Cancer a disease of the ecology of cell populations?

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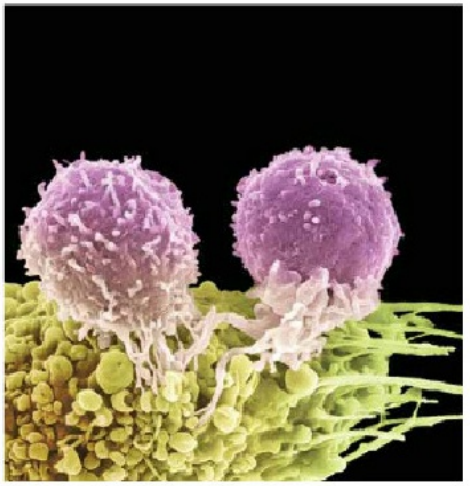

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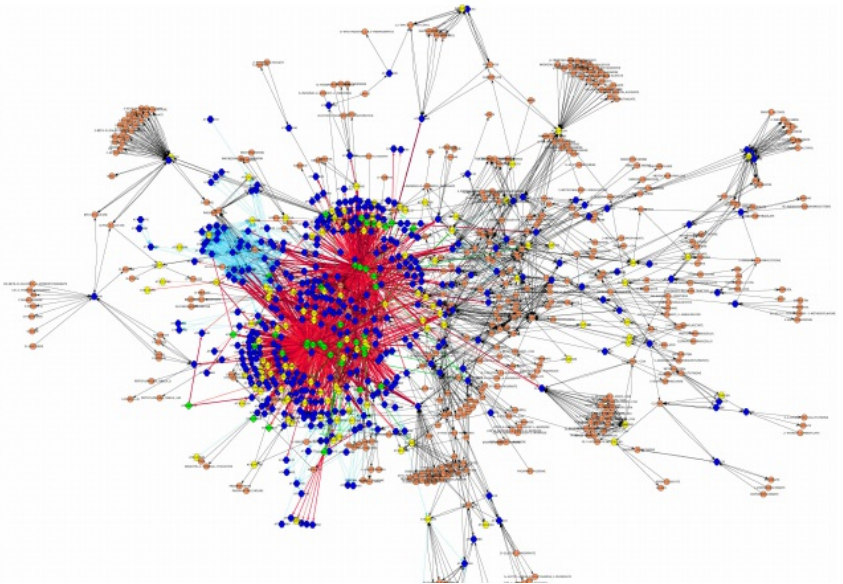
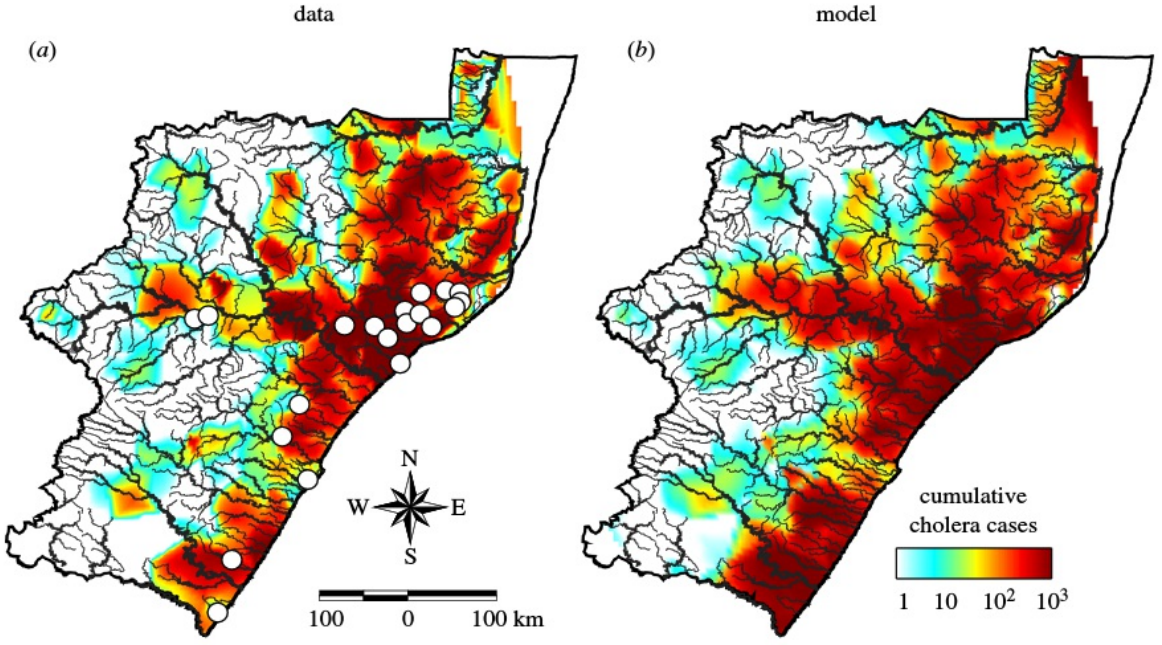
To better fight Cancer, we need to better understand the dynamical aspects of the (gene, protein, cell) interaction networks.

We need large-scale data analysis + modelling



SPREADING OF CHOLERA EPIDEMICS

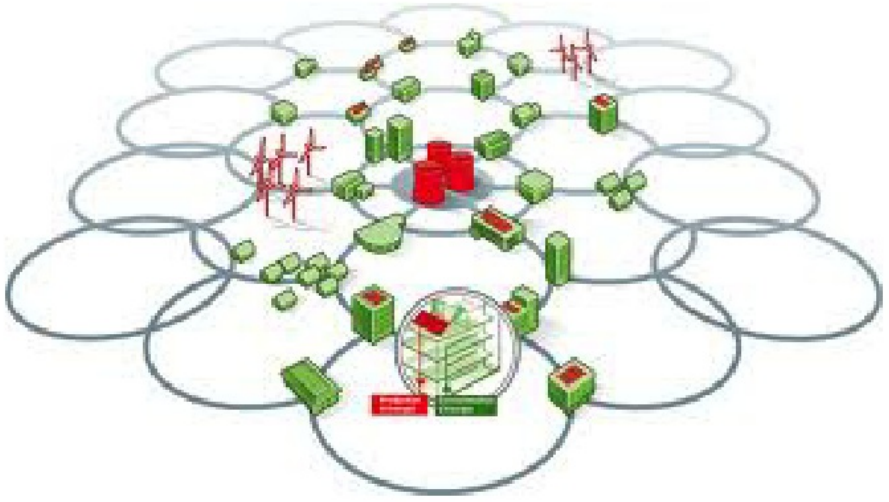


- Cholera is a waterborne disease, diffusing through water.
- How can we predict the spreading of cholera in a given geographical region?
- How can we counter-act to a rising epidemic, to stop it, e.g. by vaccination?

OPTIMAL FISHING POLICY

- Fishing alters the equilibrium of the see ecosystem.
- The number of prey and predators tend to follow a cycle at equilibrium (from many preys, few predators to few preys, many predators)
- Can we find a fishing policy that does not destroy the system, but rather stabilises it?

LOAD CONTROL IN SMART GRIDS



- Renewable energies introduce a high volatility and unpredictability in energy production.
- If the demand of energy exceeds the production, then we need to activate standard plants, to to reduce consumption by switching off devices (e.g. water boilers remotely controlled by smart meters).
- What is the optimal policy to achieve this?

AN EXAMPLE: SIS EPIDEMIC

SUSCEPTIBLE-INFECTED-SUSCEP...

$$S + I \xrightarrow{\text{inf}} I + I, \quad k_I \cdot N_S \cdot N_I$$

$$I \xrightarrow{\text{rec}} S, \quad k_R \cdot N_I$$

$$\begin{cases} \frac{d}{dt} N_I = +k_I \cdot N_S \cdot N_I - k_R N_I \\ \frac{d}{dt} N_S = -\frac{d}{dt} N_I \end{cases}$$

Outline

An high level view on CS

High level view

We will look at complex systems as systems made up of entities interacting in complex ways.

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, ...

A MAP OF COURSE TOPICS