# There’s nothing so practical than a good theory – *(Kurt Lewin)*

Mathematical models from observations to decisions

**József Baranyi**

*Institute of Nutrition, University of Debrecen, Hungary*

# Globalisation

"Today the world faces major problems. Some uppermost in my mind are

- climate change,
- food security,
- global health and making economies sustainable…."

However, … "debates are sometimes threatened by … inappropriate headlines in the media, and by those who distort the science with ideology, politics, and religion."

**Dimbleby lecture of Nobel Laurate Paul Nurse, 28. Febr, 2012**

## Mathematical developments have always been induced by demands in science, industry and business

(László Lovász, President of Hung.Ac.Sci; NetSci 2011)

| | | |
|---|---|---|
| **Land-issues** | ➔ | **Euclidian geometry** |
| **Newton's physics** | ➔ | **Calculus** |
| **Quantum mechanics** | ➔ | **Probability** |
| **Weather forecast** | ➔ | **Chaos** |
| **Economy, Ecology** | ➔ | **Game theory** |

**Now: Century of Complexity**

**Climate change, Food, Water and Energy security**
**Globalisation ➔ Science of Complexity** (System theory, Network analysis, Chaos, Sensitivity Analysis, Game theory, Risk and Uncertainty)

# Complexity

*(IT IS NOT "complicatedness")*

## Complexity has many definitions but there are some common points:

- Hard to predict; randomness is inevitable

- Emergence; at higher level of organisation, patterns emerge

- Self-organisation; patterns emerge without an external regulator

- Sensitivity to small perturbance; high degree of non-linearity

- Links between constituents are more in number, and they are more important to study, than the constituents in isolation.

# Part 1.

# Deterministic laws and randomness are both needed for life

# Fooled by the concept of “average”

An average human has one breast and one testicle…

*Des MacHale*

If you put your head in the oven and your bottom in the fridge then your average body temperature should be OK

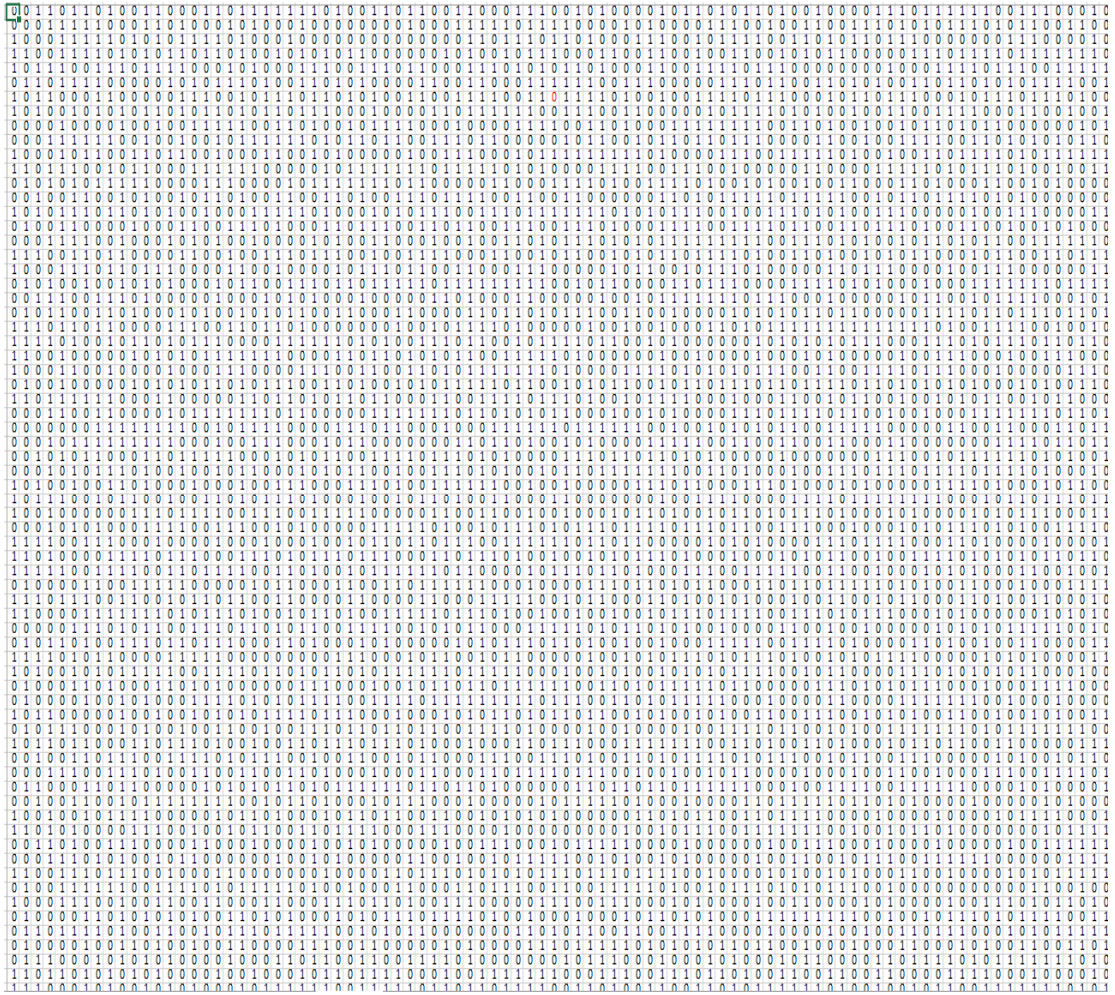
*Unknown*

# Conway: Game of Life

Two states of each cell on a sufficiently big grid: 0 and 1.
Cell-state follows local majority: that of the eight neighbours.

Consider 1 and zero as the outcome of a random vote.

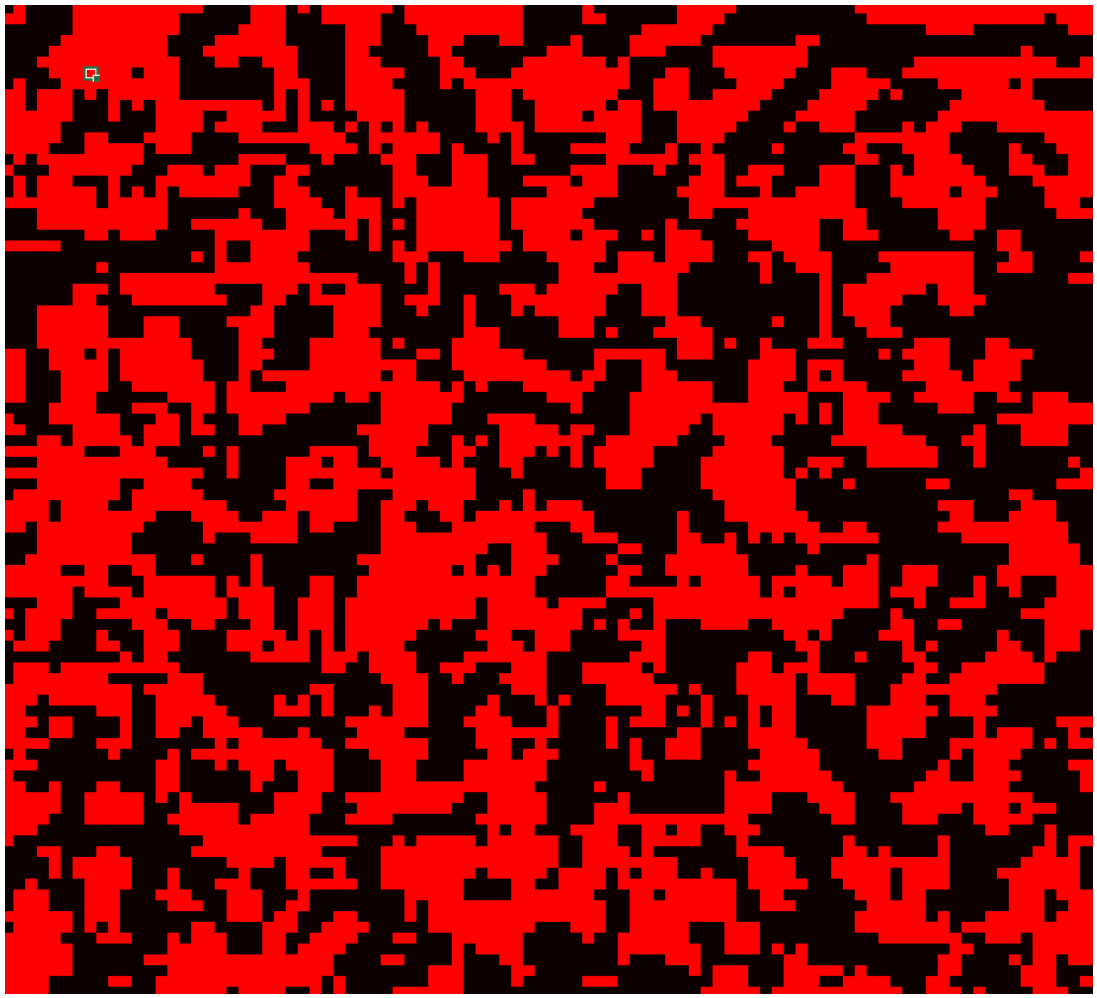
Initial distribution: p:q with 50:50% expected value.
StDev: $\sigma \sim N^{-1/2}$ .
If $N=10^6$ (one million votes) then even 51:49 % is rare.



# *Model: “local majority” drives the change*

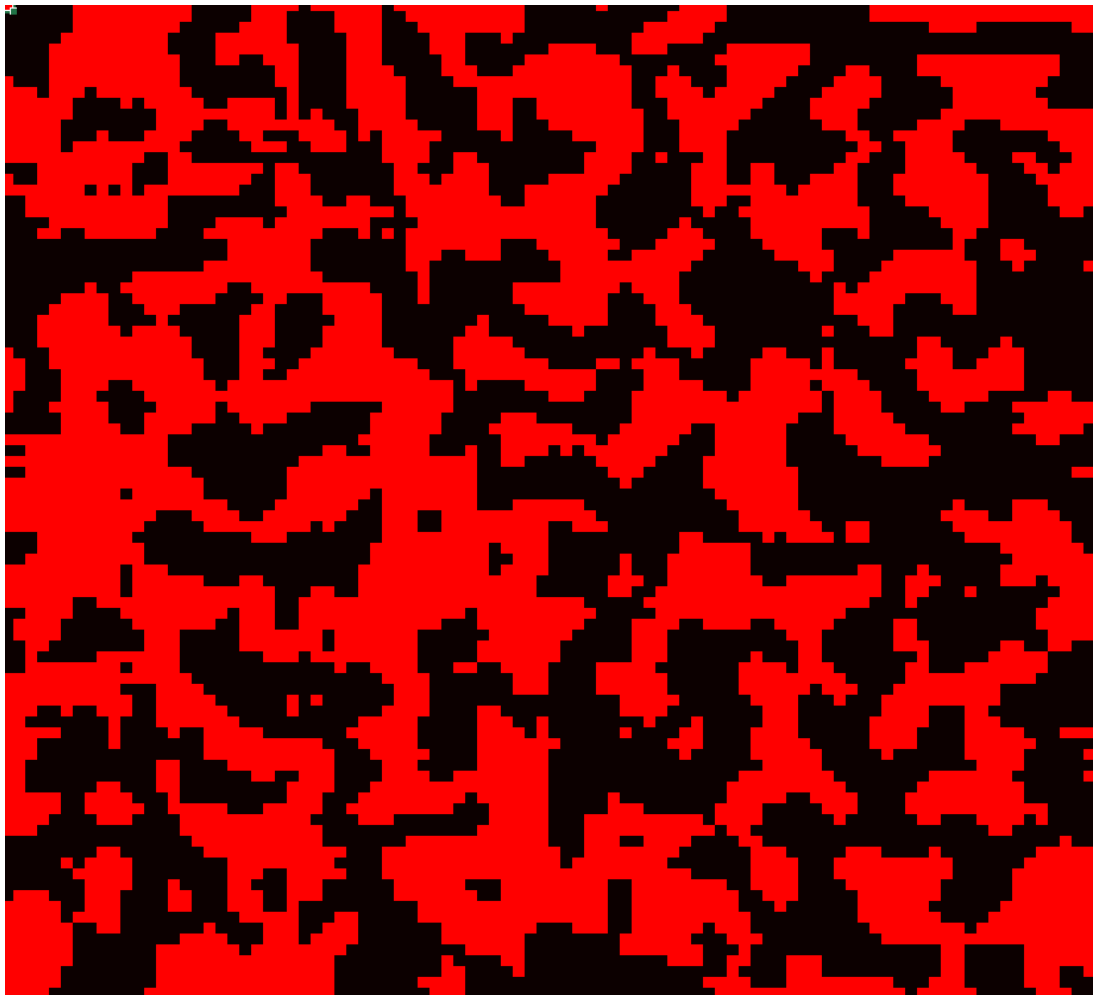
**Visualization: red=1 and black=0.**

**Initial distribution: 50-50%**



# *Model: “local majority” drives the change*

**Interaction with neighbour changes the scatter.**

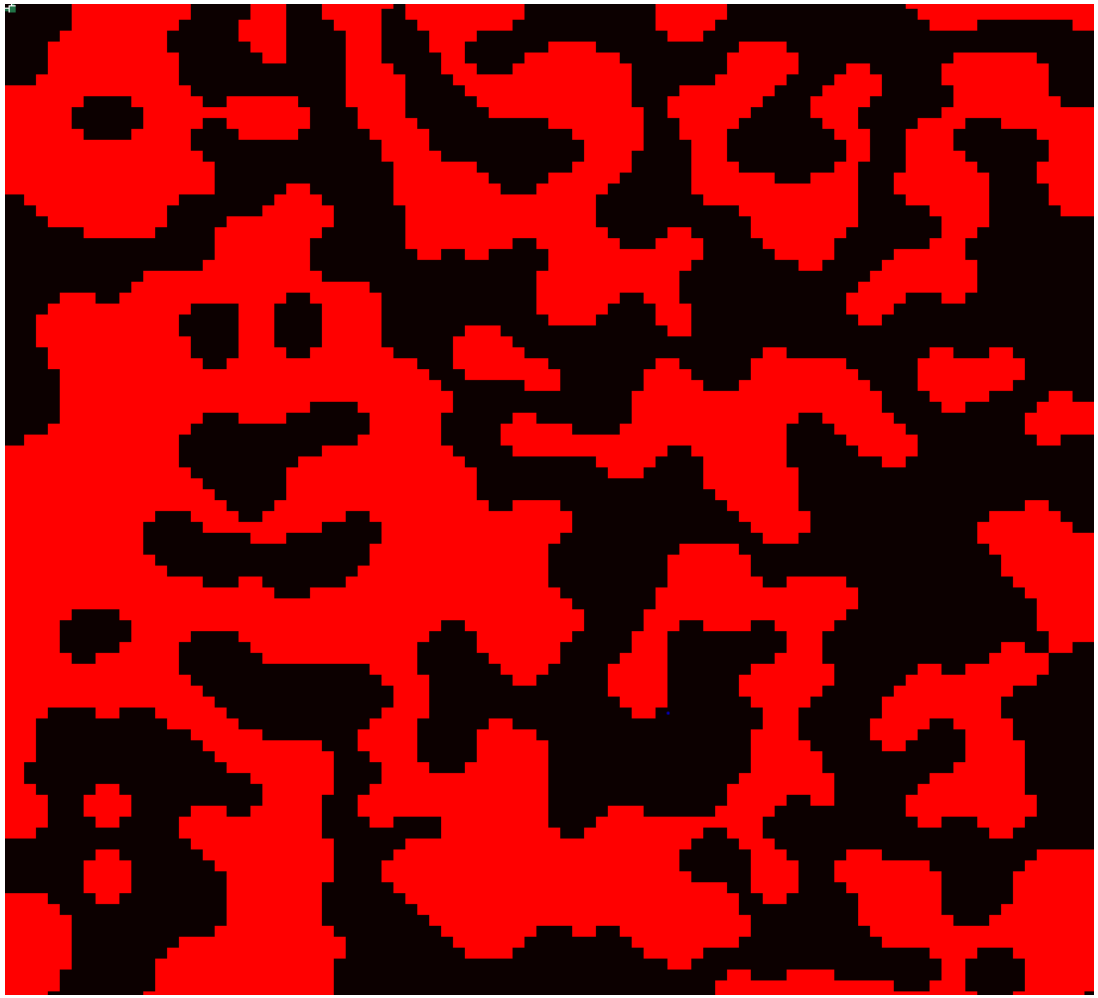


# *Model: "local majority" drives the change*

**Converges to spatial distribution with big clusters of red and black: segregation of the population converging to stable p:q proportion.**

**Expected value is 50:50% but with much bigger uncertainty than the original, upto > 10% .**

**An 52:48% ratio is a an ordinary result.**

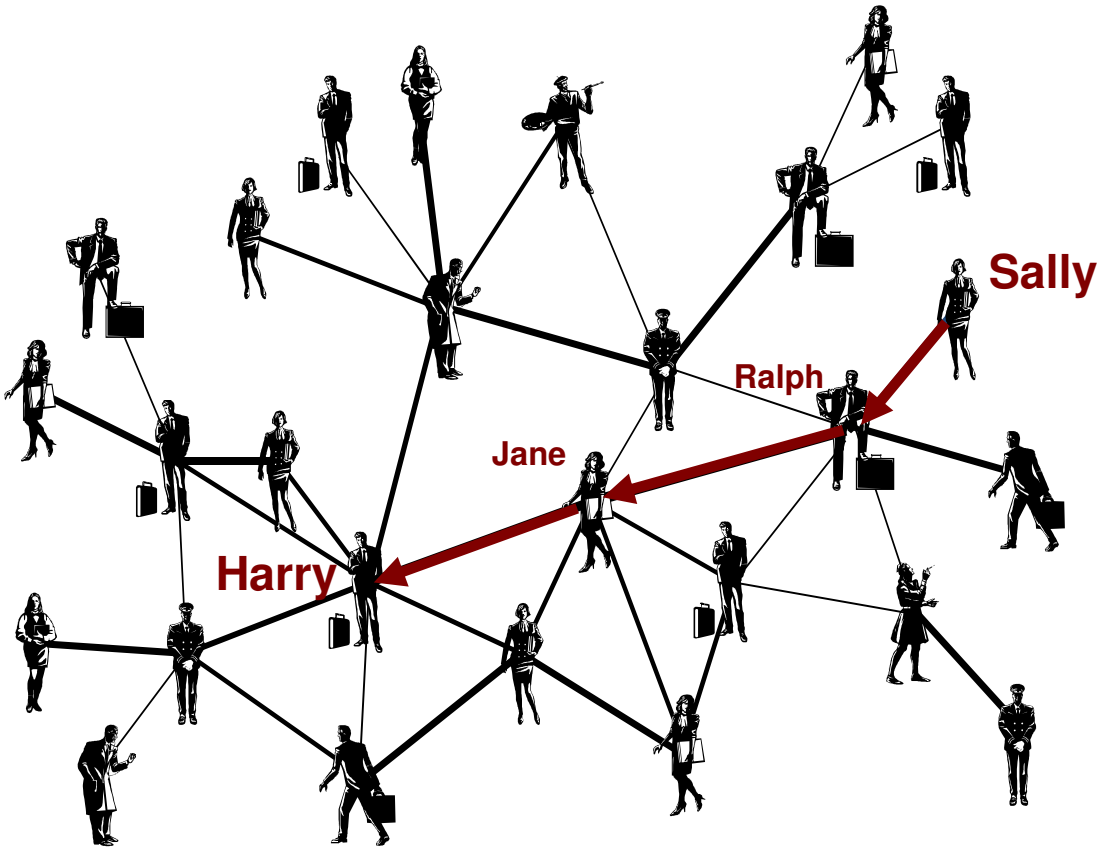


# Part 2.

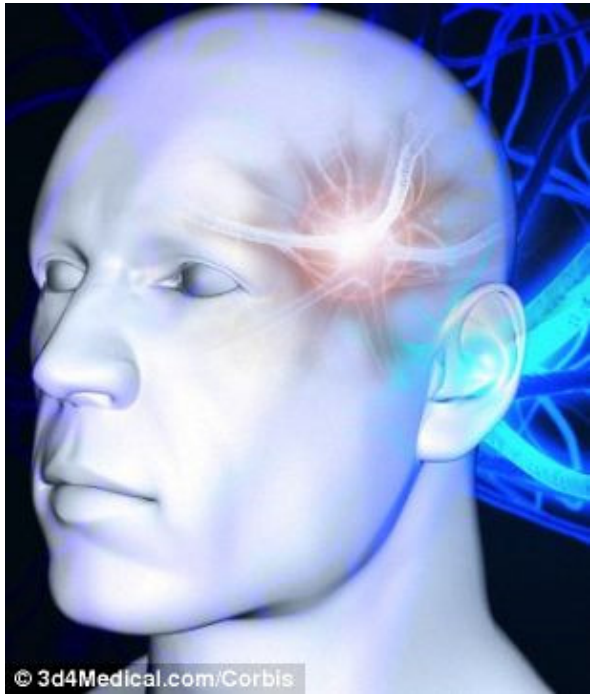
# Links and Interactions.

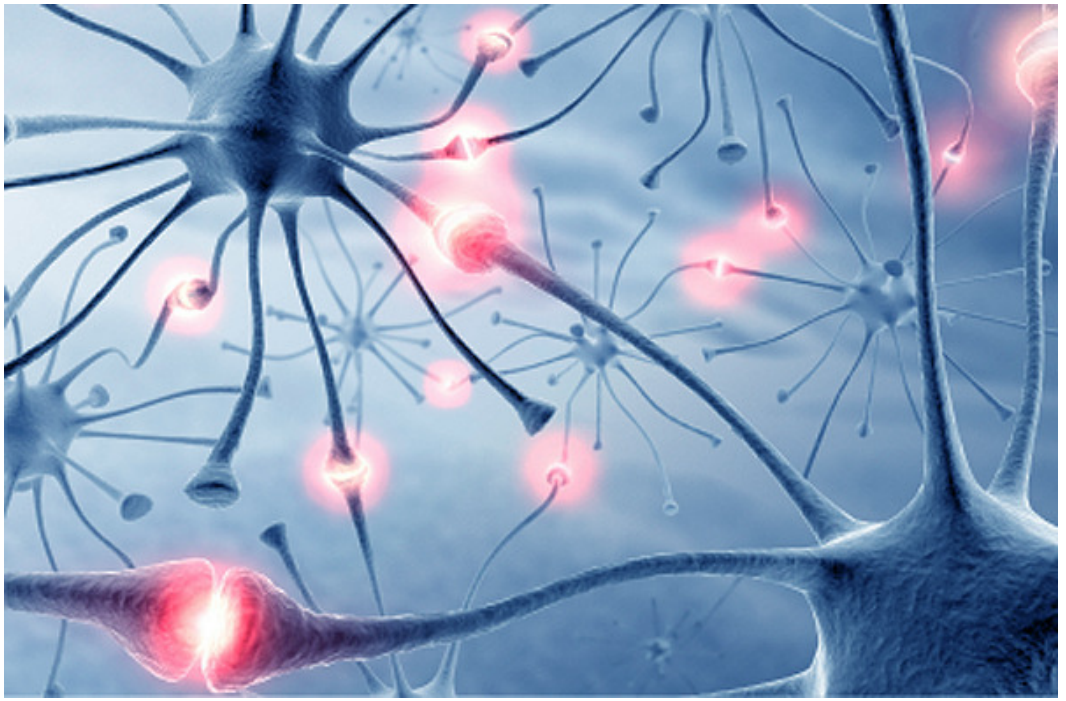
Think networks

# When Harry met Sally



# Structural and functional connections in the brain explored by network theory



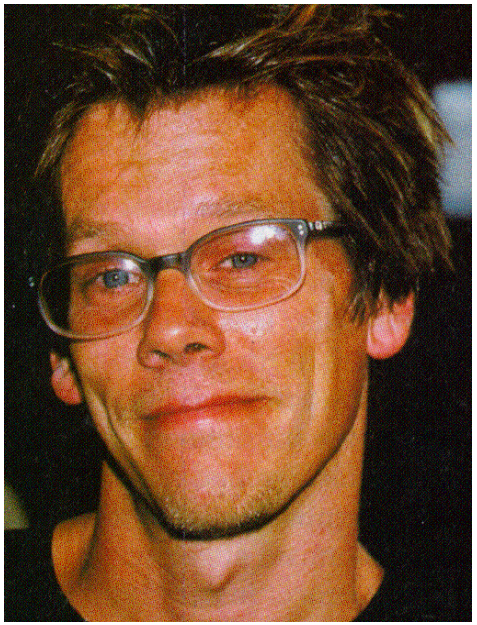
Austin Powers:
The spy who
shagged me

Let's make
it legal

**Robert Wagner**

Wild Things

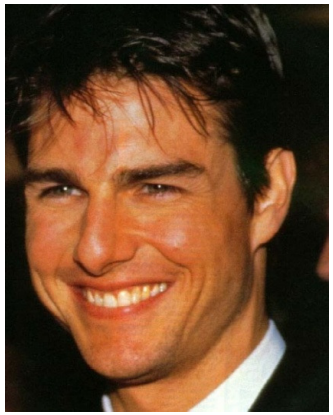
What Price Glory



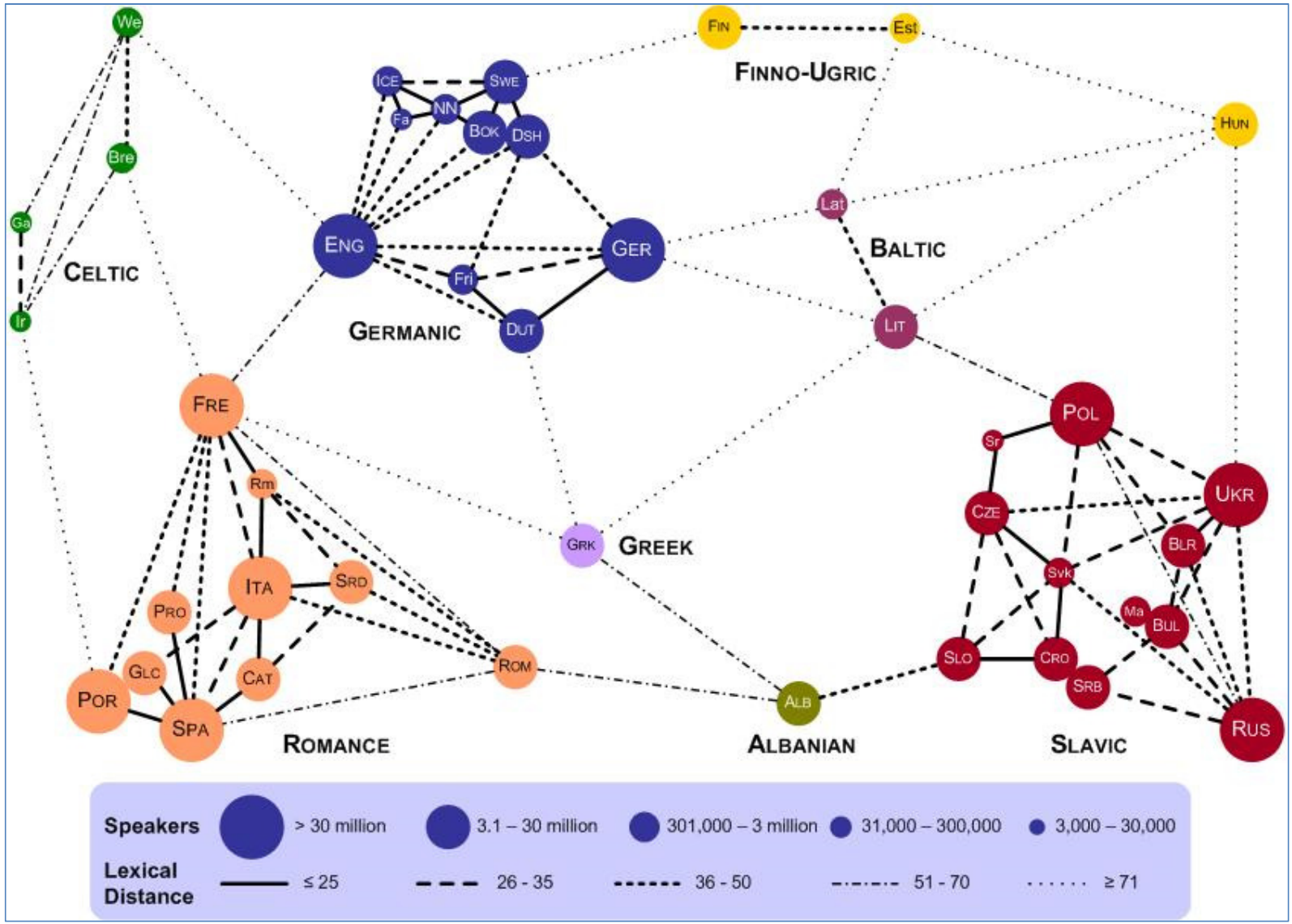
**Barry Norton**

Monsieur
Verdoux

A Few
Good Man

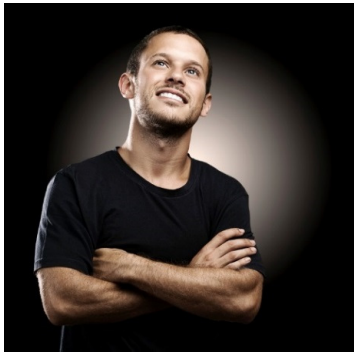


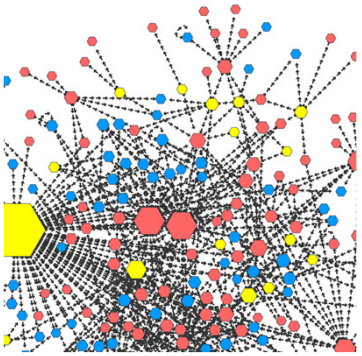
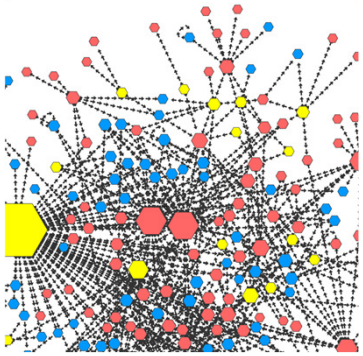
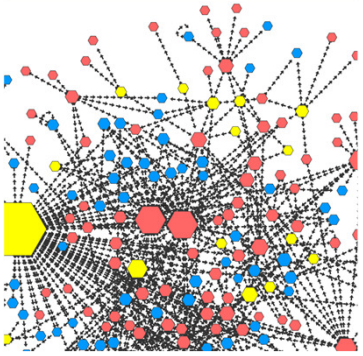
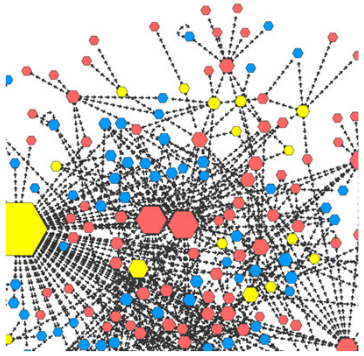
# Family ties between languages



# Interwoven networks, frequently of similar structure, at every level of life

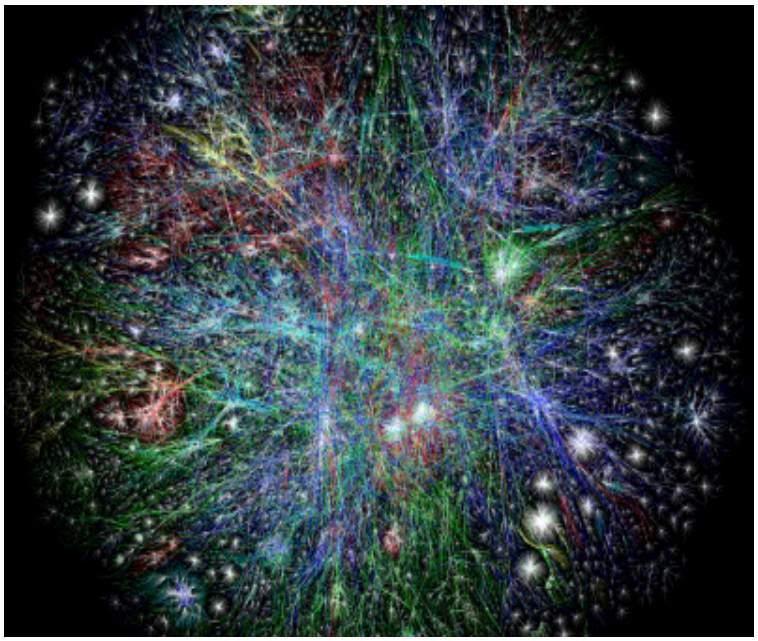




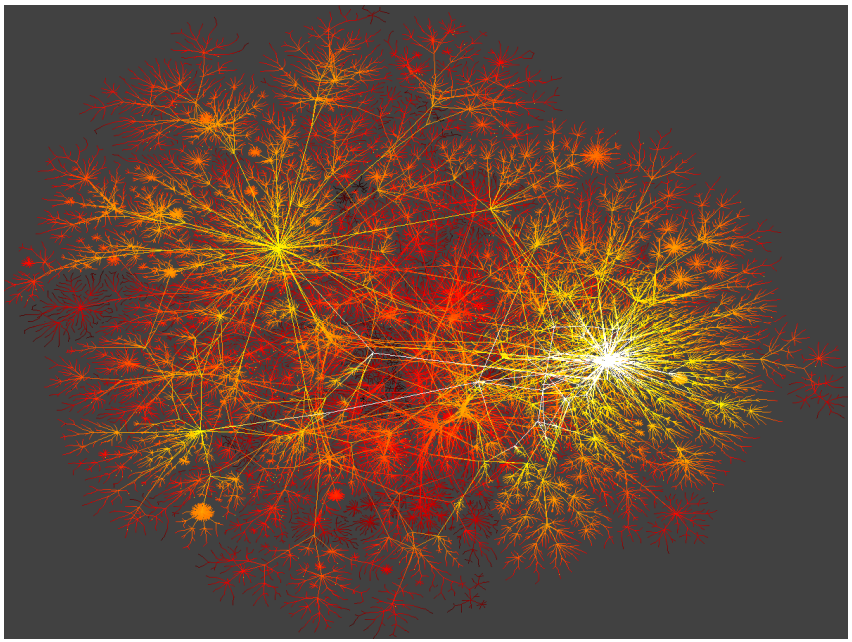
# Living in a connected world

**Internet connected by routers physically)**



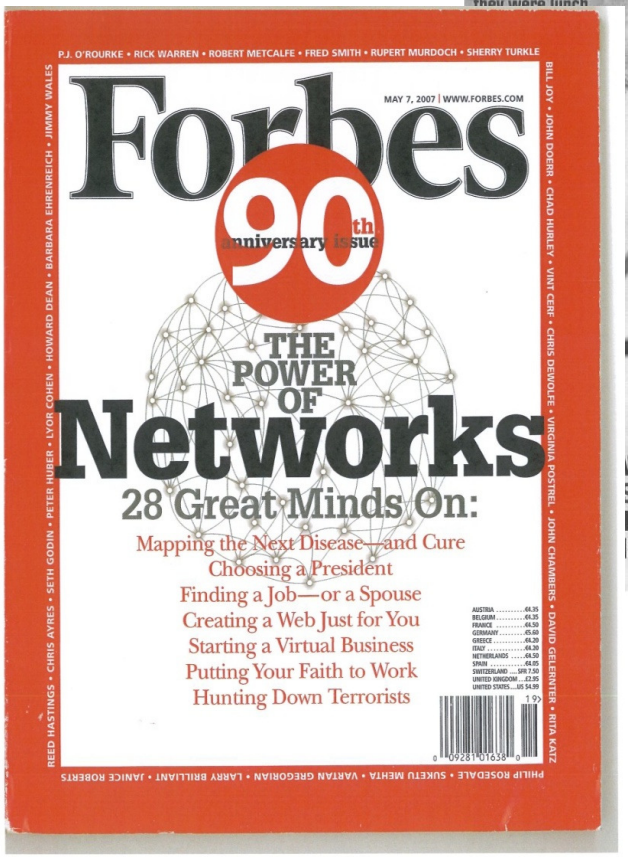
**Physical links**

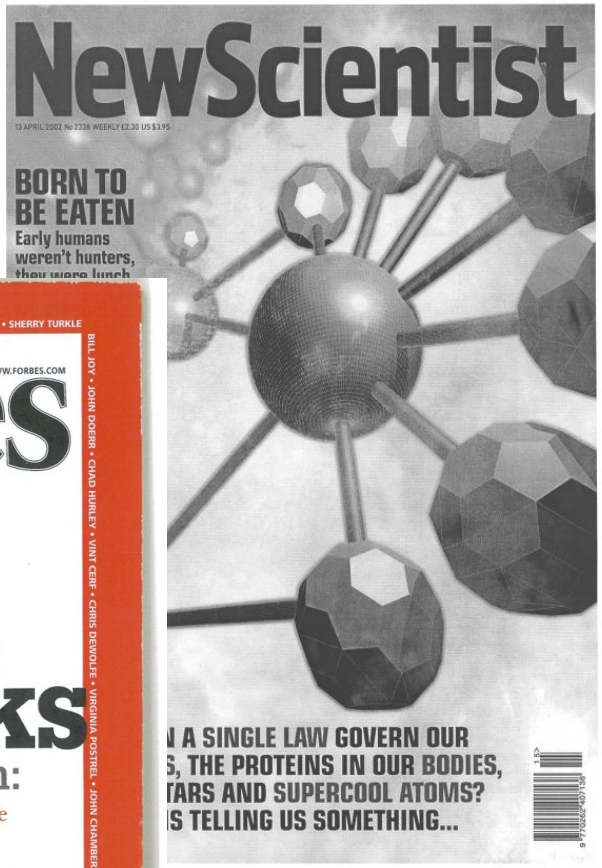
**Web-pages connected by links (URL addresses)**

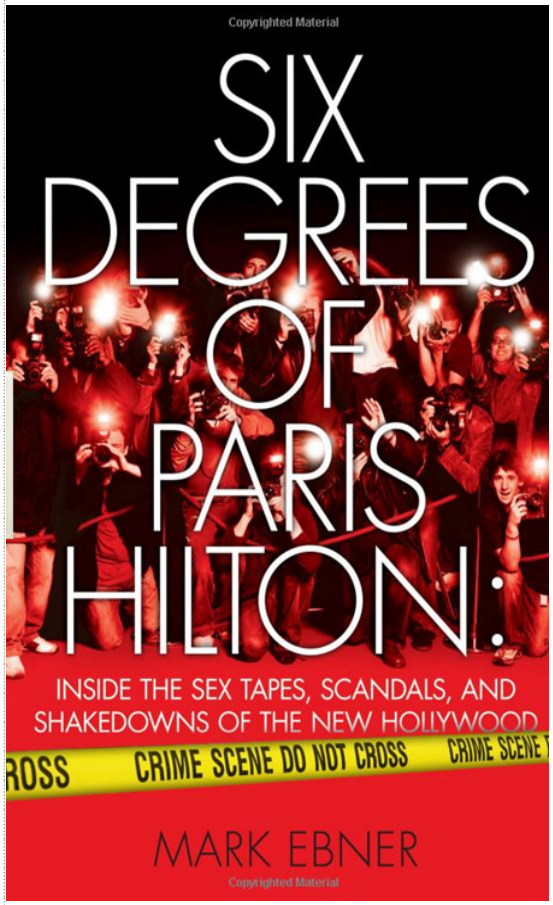


**Clicks on web pages**

**Fascination with "Six Degrees" does not decrease**



# Six Degrees of Separation, 5 May, BBC2


Documentary unfolding the science behind the idea of six degrees of separation. Originally thought to be an urban myth, it now appears that anyone on the planet can be connected in just a few steps of association.

**Six degrees of separation is also at the heart of a major scientific breakthrough; that there might be a law which nature uses to organize itself and that now promises to solve some of its deepest mysteries.**

# What is “Six Degrees of separation”?

IMDb > Six Degrees of Separation (1993)

## Six Degrees of Separation (1993) More

Photos (see all 14 | slideshow)

Own the rights?

Buy it at Amazon

Discuss in Boards

More at IMDb Pro

Add to My Movies

### Overview

User Rating: 6.9/10 8,310 votes

MOVIEmeter: Up 21% in popularity this week. See rank & trends on IMD

Director: Fred Schepisi

Writers (WGA): John Guare (play)

IMDb > "Six Degrees" Pilot (2006)

add poster

## "Six Degrees" Pilot (2006)

### Overview

User Rating: 6.8/10 34 votes

Own the rights?

Buy it at Amazon

Discuss in Boards

Add to My Movies

Update Data

Director: Rodrigo García

Writers: Raven Metzner (creator)
Raven Metzner (written by)
more

Contact: View company contact information for Pilot on IMDbPro.

TV Series: "Six Degrees" (2006)

Original Air Date: 21 September 2006 (Season 1, Episode 1)

guardian.co.uk | TheObserver

News | Sport | Comment | Culture | Business | Money | Life & style

News > Technology

## Proof! Just six degrees of separation between us

After checking 30 billion electronic messages, Microsoft researchers say the theory stands up

David Smith, technology correspondent
The Observer, Sunday 3 August 2008
Article history

Just six degrees of separation or fewer between the Dalai Lama and everyone else. Photograph: Carl de Souza/AFP/Getty Images

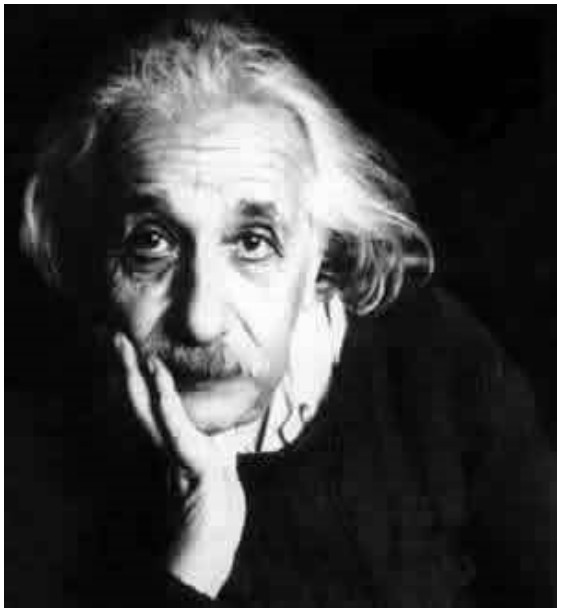
In a world of 6.6 billion people, it does seem hard to believe. The theory of six degrees of separation contends that, because we are all linked by chains of acquaintance, you are just six introductions away from any other person on the planet.

# Globalization – living in increasingly *Small-world-networks*

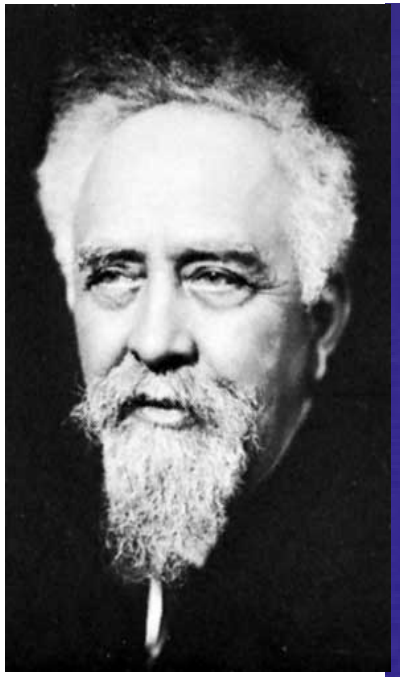

Friendship-network on Facebook, December 2011

L1

# Random walk theory

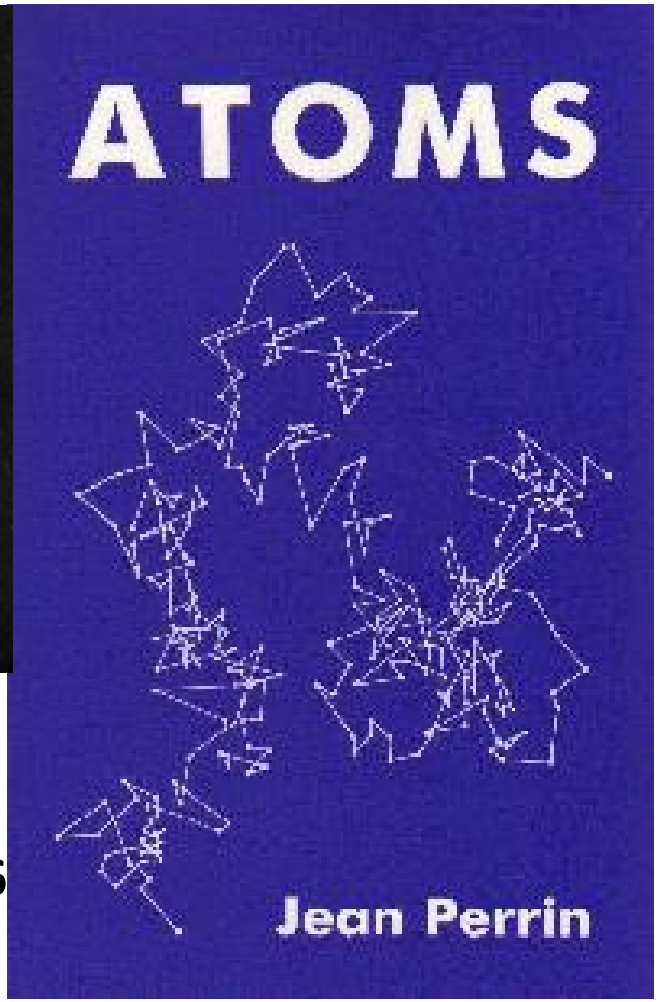


Albert Einstein,
The theory of the Brownian motion
ANNALEN DER PHYSIK (1906)



Verified by Jean Perrin

Nobel Prize, 1926



L1 Everybody seems to know one artilce that E wrote in 1905: his theory of relativty. Most people do not know that within physics he is equally famous for another article, entitled The therofy of brownian motion, in which he proposed the equations of motion for a particle that moves completly randomly in space, as a drunken sailer heading home: one step to the left, one to the right, one forward, then again to the left and so on.

But why did his conteporaries care about this little and apparently silly problem? Becouse at that time it was not clear that there are atoms at all.

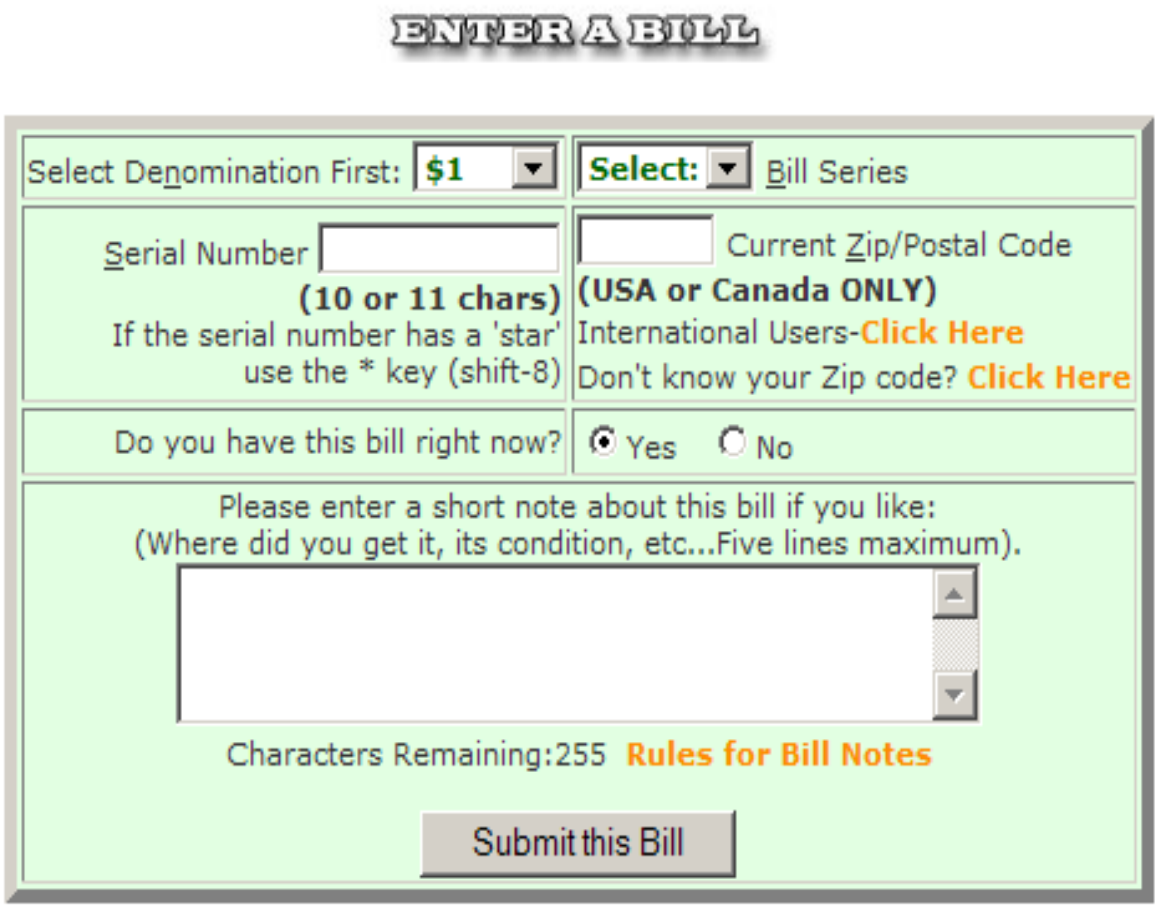
What Jean Perrin figured out is how to track the

Laszlo, 23/09/2008

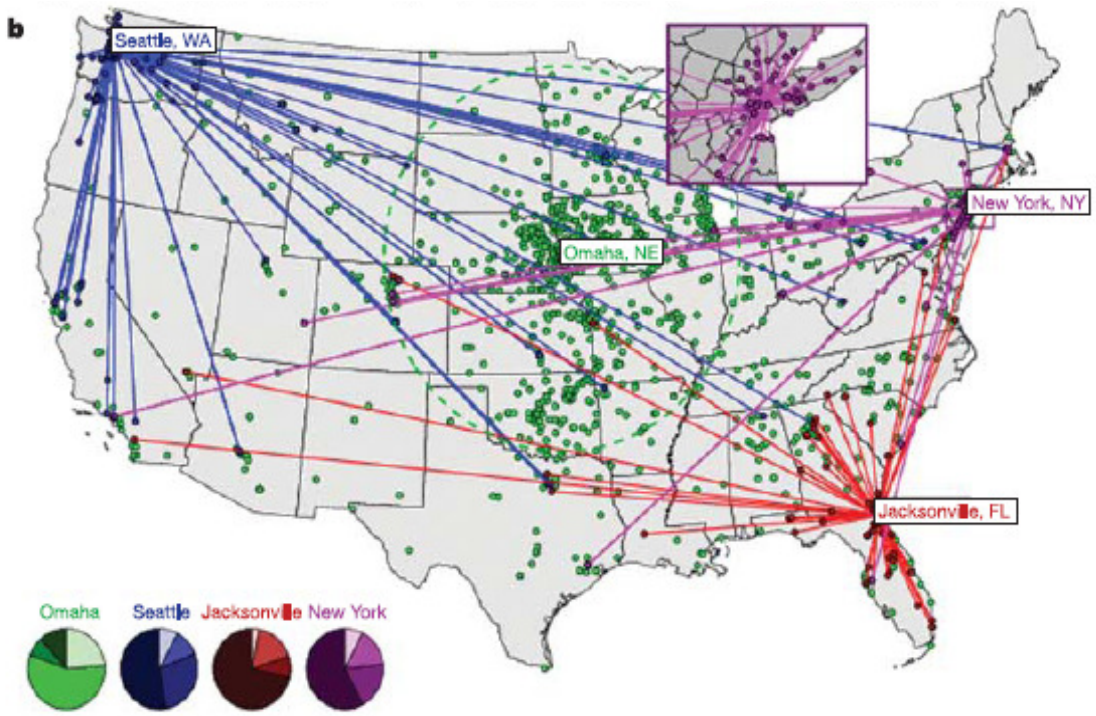

# Modelling human motion


**Brockmann, Hufnagel, Geisel: *Nature* (2006)**

# Where is George ? ➔ www.whereisgeorge.com



# Money movement ➔ like spread of epidemic



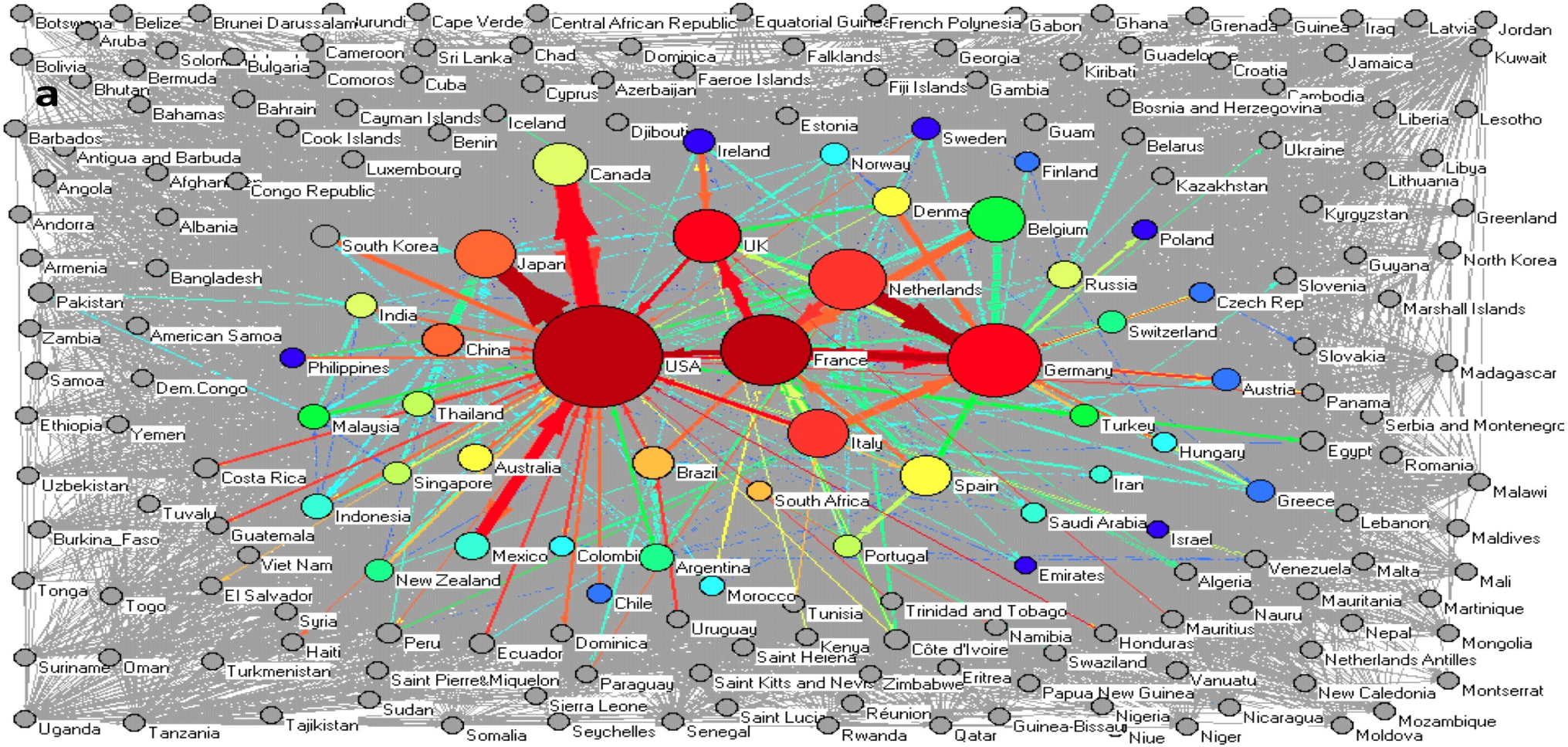
# Globalisation of Food Trade

***"The World on your Plate"***

**Chicken Kiev**

| | | |
|---|---|---|
| **Herb Butter:** | Salted butter | - Ireland |
| | garlic puree | - China, USA, Spain |
| | garlic salt | - China, USA, Spain |
| | lemon | - USA |
| | parsley | - France, UK |
| | pepper | - India |
| | water | - Ireland |
| **Chicken Breast:** | Chicken | - Ireland, Belgium UK, Thailand etc. |
| **Batter:** | Flour | - Belgium, France |
| | Water | - Ireland |
| **Bread Crumb:** | Bread crumb | - Ireland, UK |
| | Rape-seed oil | - EU, Australia Eastern Europe |

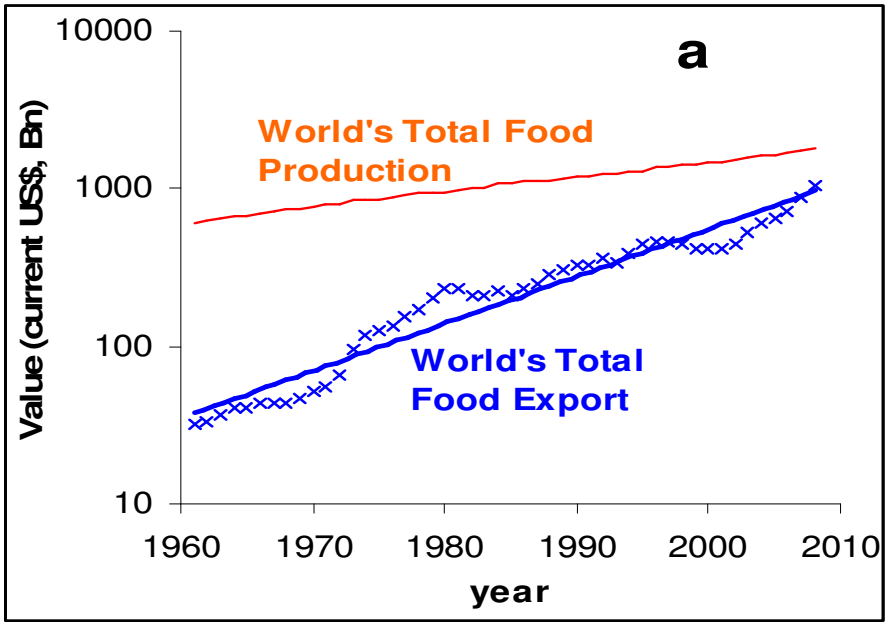
# The International Food Trade Network (IFTN)

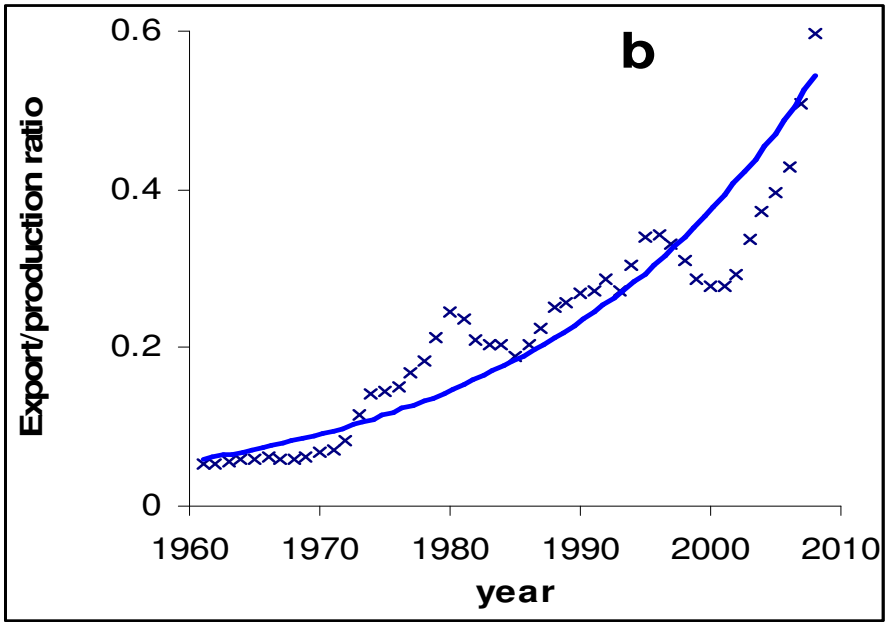



Size of nodes and thickness of links are proportional to the trade volume.

The hotter the colour the higher the betweennes centrality of the node / link (i.e. the more probable that a trade route between two randomly chosen countries go through it.

# Exponential growth of the International Food Trade Network

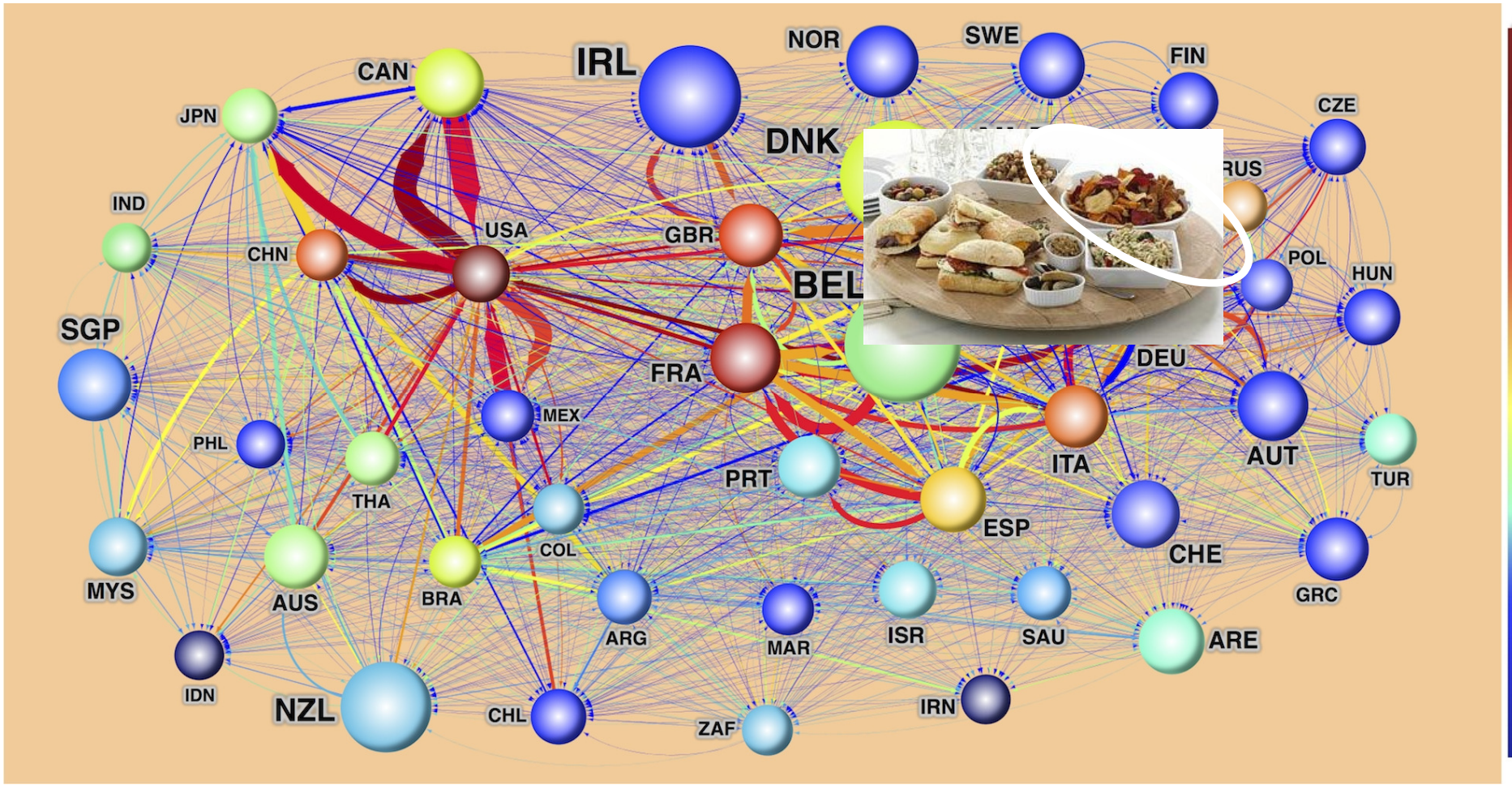



a, The world's food production doubles in ca. 30 years, while the amount of food transported on the IFTN increases by ca. 10-fold in the same time. Food ingredients arrive from a fast increasing number of countries at the consumers, shown by the exponentially increasing [world export] / [world production] ratio.
Note that the US$ inflation rate has no effect on the ratio. Data downloaded from UN databases (ComTrade).

M Ercsey-Ravasz, Z Toroczkai, Z Lakner, J Baranyi (2012); PloS One 7(5) e37810

# Backbone of the IFTN




The food-traders in Netherlands turned out to be the "*Lazy Suzanne*" of the world.

M Ercsey-Ravasz, Z Toroczkai, Z Lakner, J Baranyi (2012); PloS One 7(5) e37810

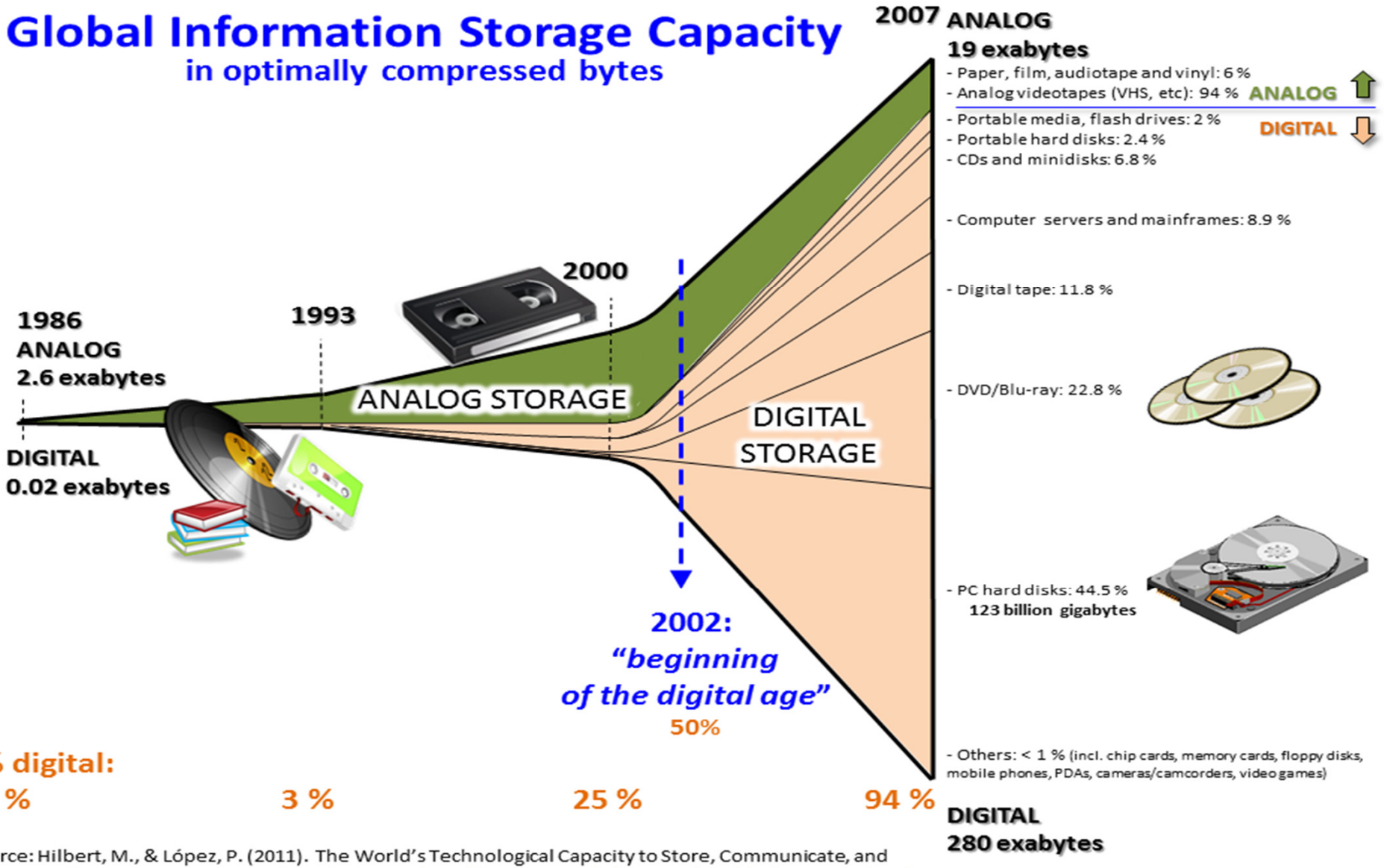
# Part 3.

# Many interacting constituents

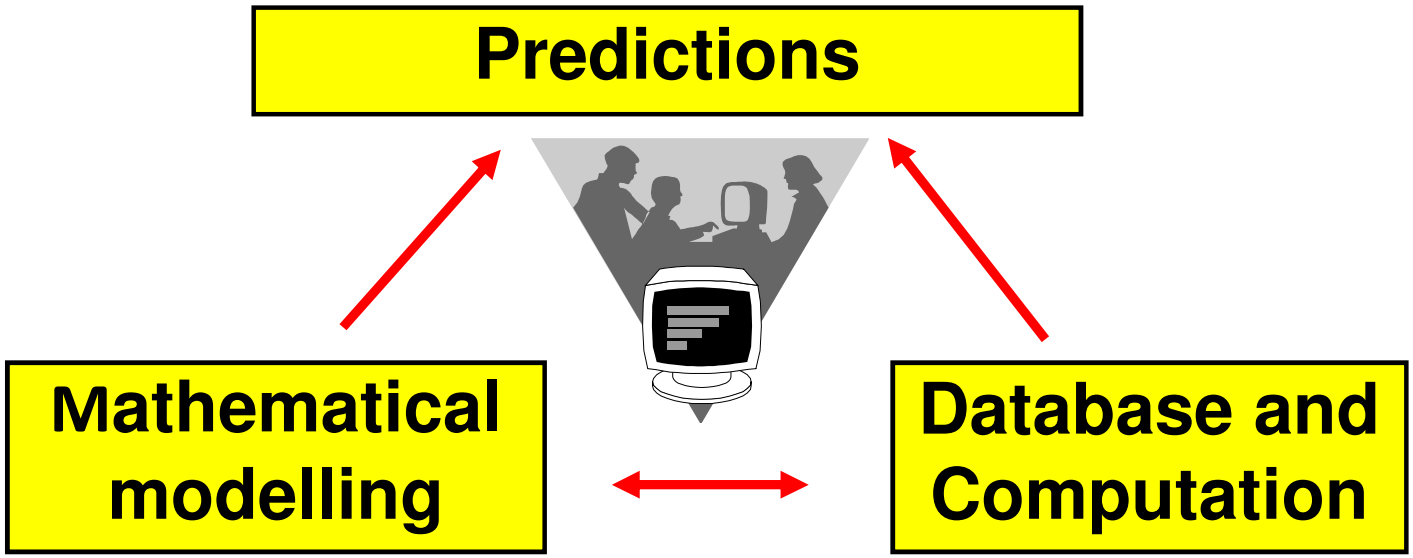
DATA SCIENCE

# Global Information Storage Capacity

## in optimally compressed bytes




Source: Hilbert, M., & López, P. (2011). The World's Technological Capacity to Store, Communicate, and Compute Information. *Science*, 332(6025), 60 –65. http://www.martinhilbert.net/WorldInfoCapacity.html


Predictions
Mathematical modelling
Database and Computation

# Look into the regulatory, metabolic and signalling network

https://www.nature.com/articles/s41540-017-0034-z



Technology Feature | OPEN

# SalmoNet, an integrated network of ten *Salmonella enterica* strains reveals common and distinct pathways to host adaptation

Aline Métris, Padhmanand Sudhakar, David Fazekas, Amanda Demeter, Eszter Ari, Marton Olbei, Priscilla Branchu, Rob A. Kingsley, Jozsef Baranyi & Tamas Korcsmáros



Subjects: Biochemical networks, Computational biology and bioinformatics

Journal: *npj Systems Biology and Applications* **3**, Article number: 31 (2017)

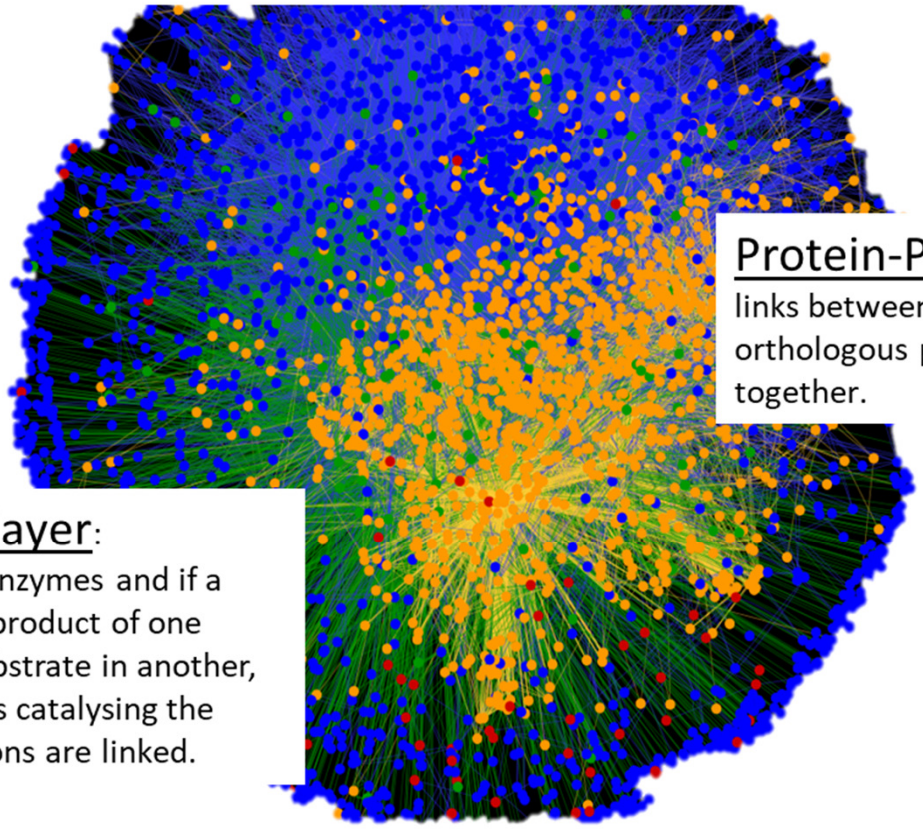
DOI: doi:10.1038/s41540-017-0034-z

Download Citation

# SalmoNet

## Regulatory network:

Regulatory links represent binding of TF to gene promoters (undirected links).

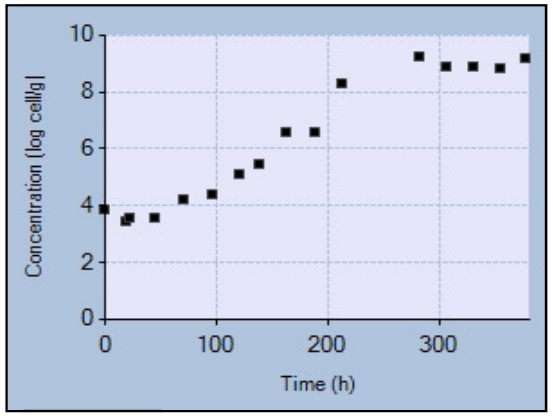


**Protein-Protein Interactions:** The links between proteins represent Salmonellae orthologous proteins of *E. coli* which interact together.

**Metabolic layer:**
The nodes are enzymes and if a metabolite is a product of one reaction and substrate in another, the two proteins catalysing the different reactions are linked.

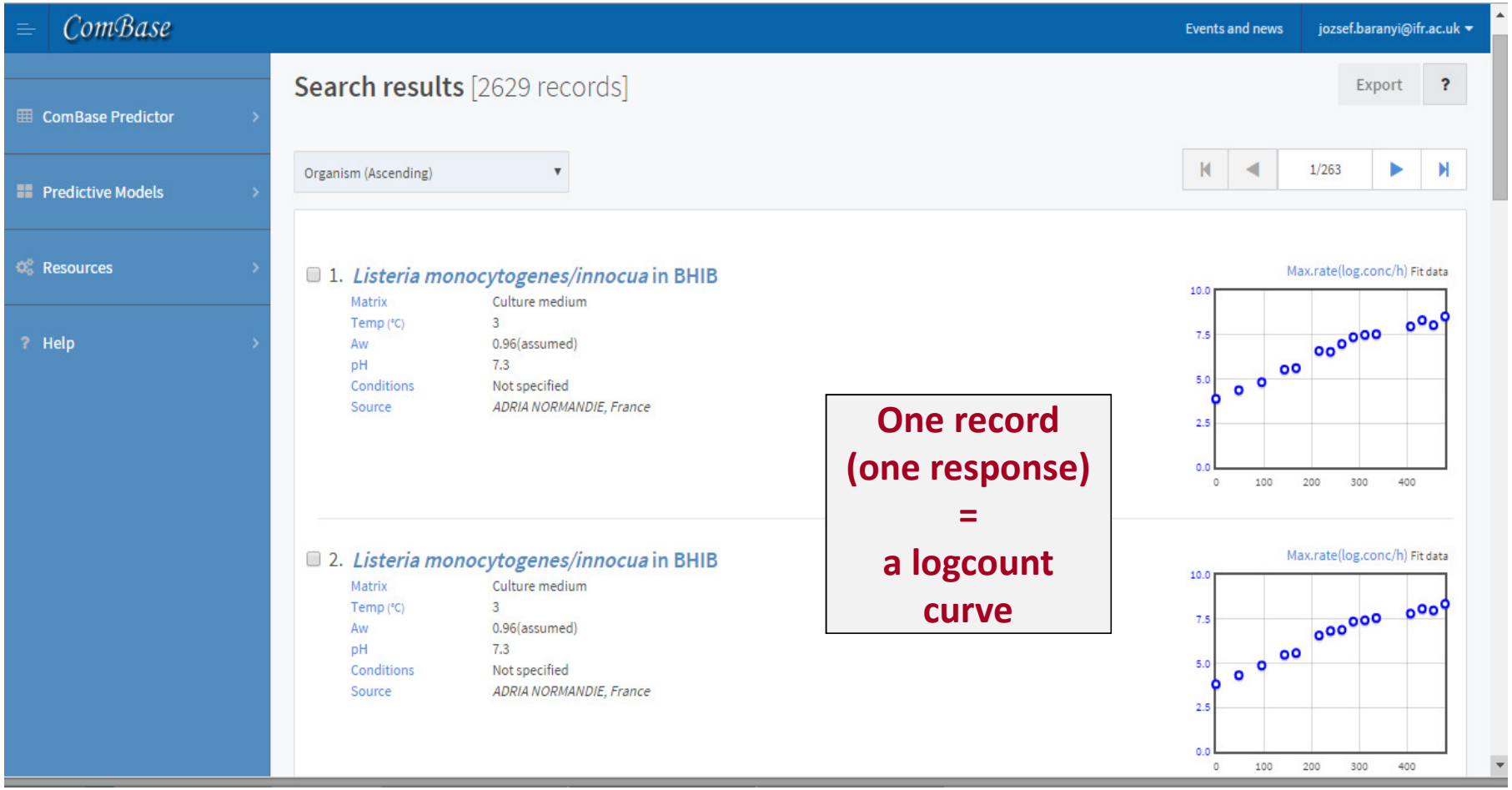
(http://salmonet.org/)

# Collecting observations in a systematically organised database (www.combase.cc)




- **Organism, data source,** *material & methods*
- **temperature, pH, water availability, atmosphere composition, preservatives**
- **observation time, specific rate**
- **logcounts, comments**

# Retrieving records specified by user-



# Display selected records

First | Back 10 | Previous | Next | Forward 10 | Last

[20/366 matches]

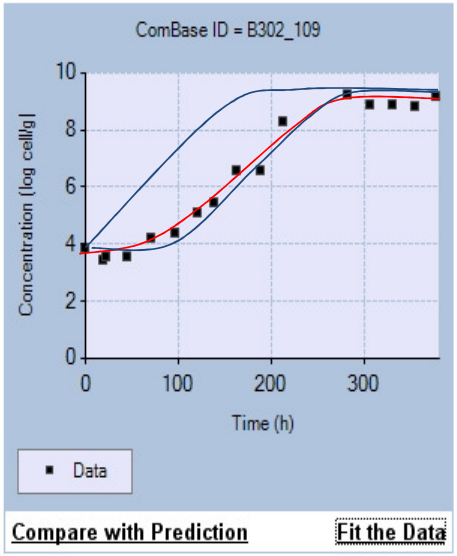
Download B302_109 to CSV

## Record Details

| | |
|---|---|
| Organism: | *Escherichia coli* |
| Food type: | Culture medium (In: broth) |
| Temperature: | 10 °C |
| pH: | 6.9 |
| Water activity: | 0.986 (assumed) |
| NaCl: | 2.5 % |
| Maximum Rate (log10(CFU/h)): | See data |

Conditions:

Carbon-dioxide in the environment(%):60, Sodium chloride in the environment(%):2.5




Compare with Prediction | Fit the Data

## Record Data

| Time (h) | log cell/g |
|---|---|
| 0.00 | 3.840 |
| 18.92 | 3.440 |
| 22.78 | 3.590 |
| 44.77 | 3.570 |
| 70.00 | 4.240 |
| 96.10 | 4.400 |
| 119.73 | 5.120 |
| 138.23 | 5.470 |
| 162.80 | 6.610 |
| 187.52 | 6.610 |
| 211.77 | 8.320 |
| 282.40 | 9.260 |
| 306.60 | 8.900 |
| 330.75 | 8.910 |
| 354.67 | 8.860 |
| 377.18 | 9.170 |

Source:

Food Standards Agency funded data generated at Institute of Food Research, UK

Further Specifications:

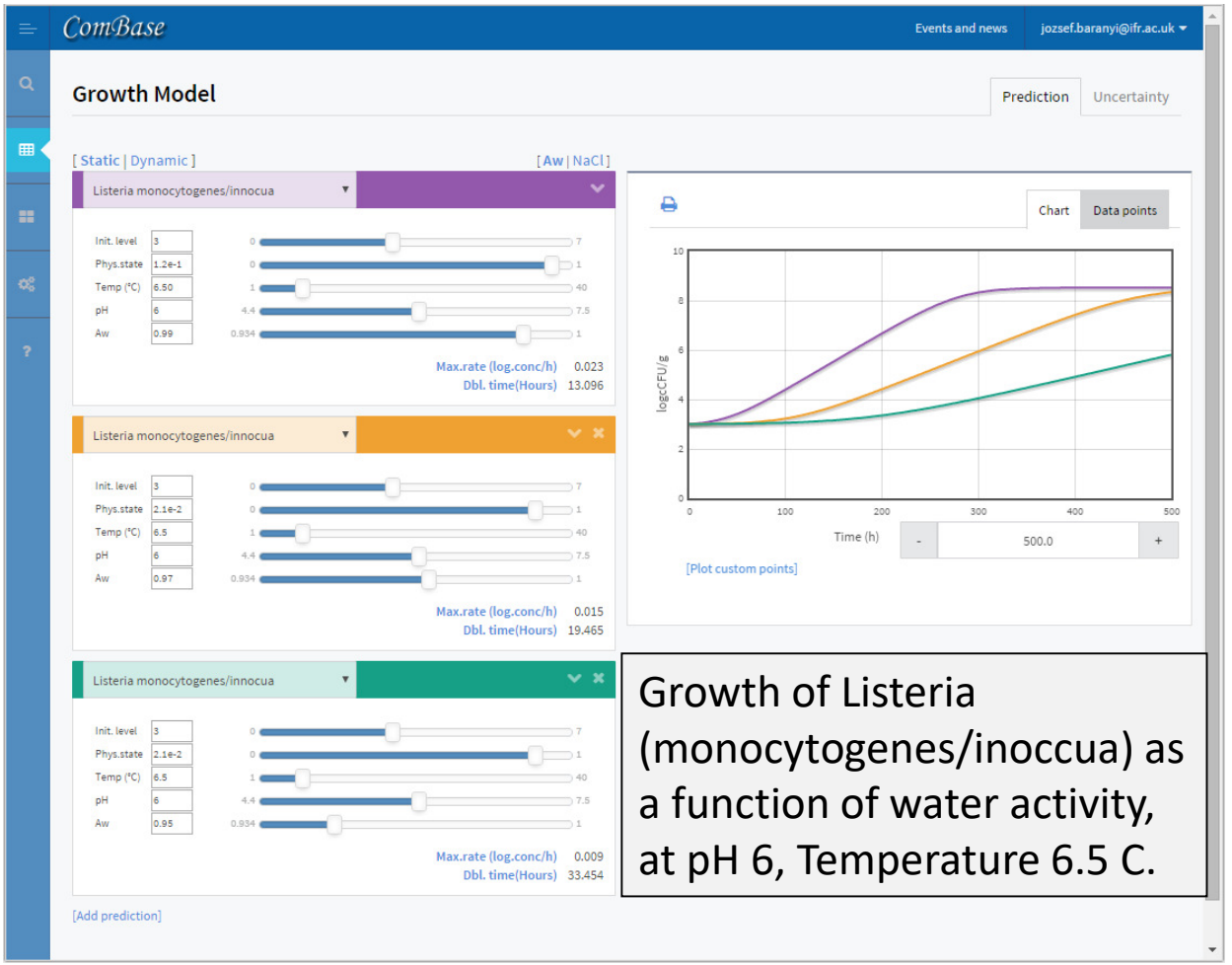
Serotype(s): O157:H7, Strain(s): NCTC12079 W2-2 505-B 204-P. Mixed_strains. Measurement by colony counts.

Details:

Growth of Escherichia coli O157:H7 in presence of CO_2. Strains: NCTC 12079, W2-2, 505-B and 204-P. Media: Tryptone soya broth (CM129)Inocula: Organisms were grown in 10 ml of medium overnight and subcultured twice more (a total of 3 passages). Cultures were mixed, diluted and added to the experimental media (90 ml of broth inoculated with 1 ml of inoculum prediluted to ca. 10^5 cfu/ml). Sterile membrane pads of 47 mm diameter were

# ComBase Predictor to study the effect of environment on bacterial growth

Confidence in prediction is boosted by the access to observed data and the tools to compare them.




Growth of Listeria (monocytogenes/inoccua) as a function of water activity, at pH 6, Temperature 6.5 C.

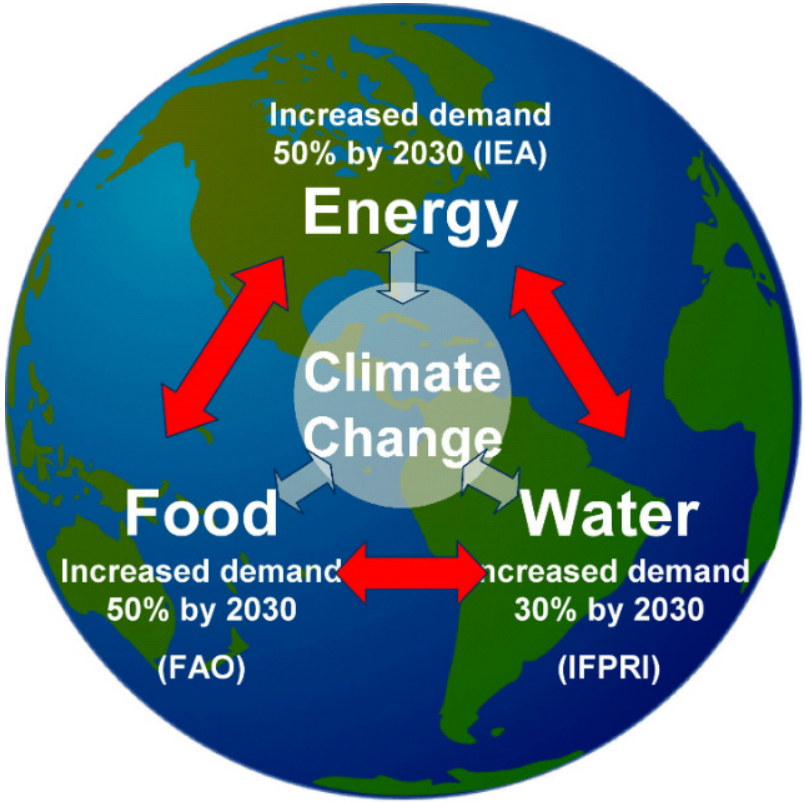
# ComBase seminars and workshops

# Part 4.

# Extreme sensitivity, Chaos

# Interconnected world

*Global issues - 2030*




John Beddington
UK Government Chief Scientist, 2012

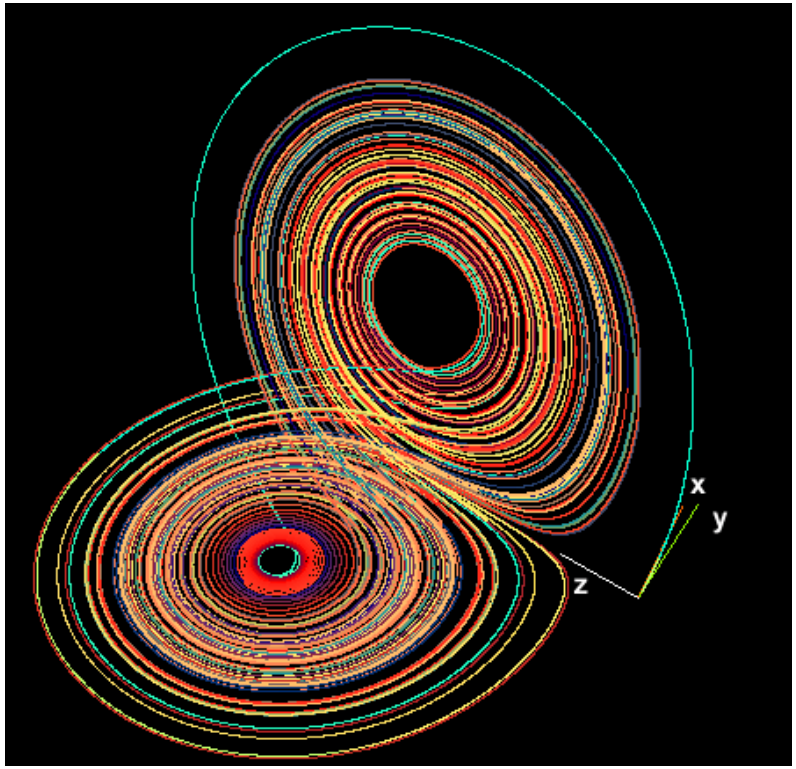
To tackle, make use of

- IT tools explosion
- Network science
- Complexity science
- Multi-disciplinary collaborations

FOOD is especially suitable to utilize progress in the above

# A famous, inherently chaotic problem

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \sigma(y - x),$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = x(\rho - z) - y,$$
$$\frac{\mathrm{d}z}{\mathrm{d}t} = xy - \beta z.$$




A three-dimensional trajectory, that can be chaotic for certain values of $\sigma$, $\rho$ and $\beta$.
Links to weather forecast.

*Edward Lorenz accidently found a chaotic system in the 50-s, when testing his model for weather forecast (of course with very many variables). Then, in 1963, he reduced it to a minimal system that can still show the chaotic behaviour; see above. This is the birth place of the Butterfly-effect.*

## Increasing noise and dispersion ending up with Pattern

https://www.youtube.com/watch?v=R6NnCOs20GQ

*Randomness produces deterministic patterns*

- Law of large numbers

***Deterministic laws can also produce random events***

- Feed-back
- Interactions