

Spatial simulations in biology and social sciences

Toward a comparative epistemological analysis

Franck Varenne – Associate Professor of Epistemology
Normandy University (Rouen) - franck.varenne@univ-rouen.fr

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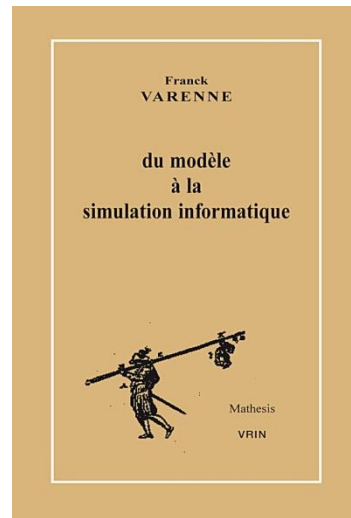
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 - One of the main results: the growing importance of the explicit representation of space and of complex spatial relations

Outline of the Talk

- Part I- A first case study : virtual developmental biology and agronomy
- Part II- Toward the notion of simulation
- Part III –Examples of integrative spatial simulations in biology
- Part IV- On some spatial simulations in social science
- Conclusions

**PART I- THE 1ST CASE STUDY : VIRTUAL
DEVELOPMENTAL BIOLOGY AND AGRONOMY**

- A case study: architectural modeling of vegetative plants in agronomy (source: ***Du modèle à la simulation informatique***, Paris, Vrin, 2007 ; ***From Models to Simulations***, Routledge, to appear in 2018).



- Result: During the 40 last years, this modeling has passed through 3 successive phases: pluriformalization, 4D simulation and remathematization of simulations

Content of the first part of the talk

The scansion of this history

- I- 1st step : Pluriformalization of growing vegetative plants (1974-1979)
- II- 2nd step: 4D simulations (1980-1998): role of OOP
- III- 3rd step: Remathematization of complex simulations (since 1998)

I- 1st step : Pluriformalization of growing vegetative plants (1)

- **Context and motivation of scientists:**
 - Modeling and improvement of Coffee tree fructification in a French research institution in Agronomy (IFCC, then the CIRAD) based in Ivory Coast (West Africa) during the 70's
 - There was a need to predict fructification very precisely in order to select the better clones of coffee tree

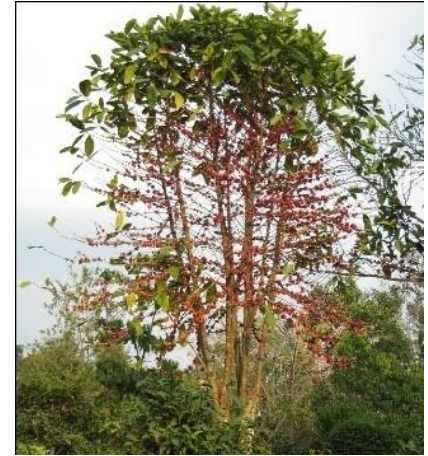


A coffee tree - Source : AMAP

I- 1st step : Pluriformalization of growing vegetative plants (2)

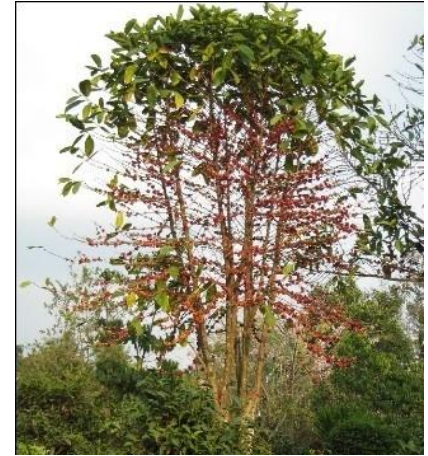
- **Some Limits of Biometry and Allometry**

- 1974: Philippe de Reffye showed that the use of traditional biometric tools such as multivariate statistics failed to predict fructification of coffee trees (“cherries” then “beans”)



- He rediscovered that the fructification of a coffee tree depends heavily on the **topology of the whole tree** (= configuration and mutual arrangements of vegetative organs), not on its geometry (known since 1921: firstly observed by J.H. Waring on the apple tree (1921), then clearly recognized by J.H. Beaumont (1938) (Hawaiï)).

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- Hence, fructification is not a linear function of the masses of the whole organism or of some of its organs (no allometry i.e. power-law : $y = a \cdot x^b$).
- Then, contrary to the production of wood, e.g., it depends on the primary growth of the vegetative plants (cell division and lengthening of new cells, branching), not on its secondary growth (growth in thickness of organs, increase in diameters of axes)

I- 1st step : Pluriformalization of growing vegetative plants (3)

- **Back to Botany: the notion of Architectural Model (Nozeran, Hallé, Oldeman, Tomlinson)**
 - « **vegetative architecture** » of vegetative plants (Hallé-Nozeran - 1964) = all its structuro-morphological features, i.e. its spatial configuration due to axes and vegetative organs (≠ latex, pilosity...)
 - « **architectural model** » (Hallé-Oldeman - 1967) = « successive architectural phases of a tree » ; « inherent growth strategy of the plant » (Oldeman, 1974). Oldeman was against the hegemony of statistical morphometry which overlooked the architecture (the bearing of trees) by grouping axes by types regardless to the whole topology of the tree.

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 - ≠ *Urpflanze* (Goethe), “seminal morphè”.
 - The AM is a sequence of elementary choices in buds, partially stochastic, and leading to a stable and genetically determined statistical phenotype. Plant Growth is not a metamorphosis (continuous topological transformation, ≠ René Thom).
 - ≠ Type of Linnaean taxonomy because inter-specific.

I- 1st step : Pluriformalization of growing vegetative plants (4)

- **Limits of Botany:**

In Hallé, Oldeman, Tomlinson (*Tropical Trees and Forest: an Architectural Analysis*, Springer, 1978) and again *in* Hallé (2004), an AM appears as a **graphico-verbal model**, because it is a combination of 4 series of heterogeneous features :

- 1) The **type of growth** (rhythmic or continuous) ;
- 2) The **branching structure** (presence or absence of ramification ; sympodial or monopodial ramification ; rhythmic , continue or diffuse ramification) ;
- 3) **Morphological differentiation of axes** (orthotropy or plagiotropy) ;
- 4) **Positions of flowers** (terminal or lateral).

- **Around 24 different Architectural Models have been observed**

- **Limit of such a botanical concept from the standpoint of agronomy:**

How to formalize and quantify an Architectural Model?

Examples of elementary graphical symbols and architectural models

(source: Hallé – 1979)

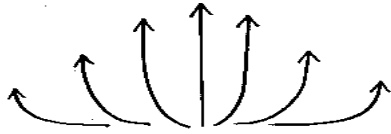


Fig. 1 — Axes verticaux, à rôle d'exploration.

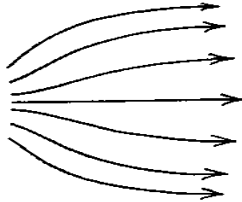


Fig. 2 — Axes horizontaux, à rôle d'exploitation.

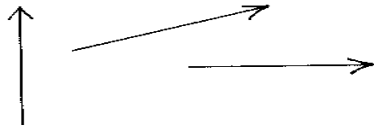


Fig. 3 — Axes non ramifiés.

Elementary symbols

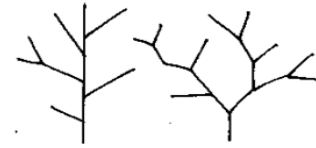


Fig. 4 — Systèmes ramifiés.

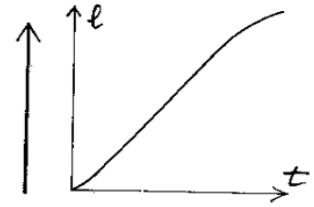


Fig. 5 — Axe à croissance continue.

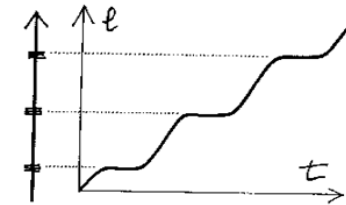


Fig. 6 — Axe à croissance rythmique (rythme endogène puisque les conditions sont constamment favorables à la croissance).

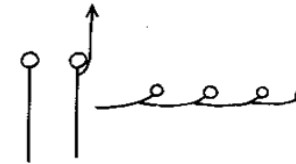


Fig. 7 — Sexualité terminale arrêtant la croissance (relais possibles).

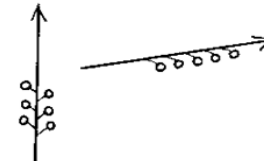
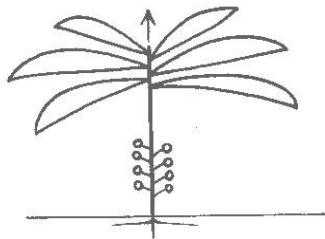
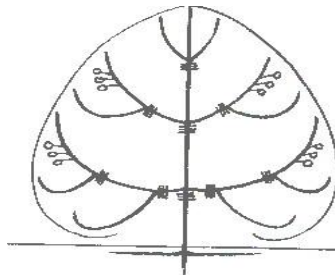


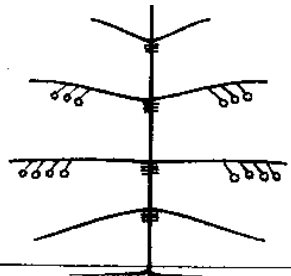
Fig. 8 — Sexualité latérale permettant une croissance indéfinie.



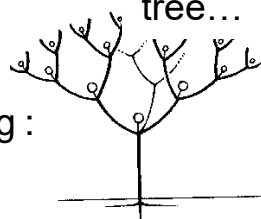
Corner : palm tree...



Rauh : oak...



Massart : fir tree...



Leeuwenberg : frangipani tree...

Architectural Models

I- 1st step : Pluriformalization of growing vegetative plants (5)

- **De Reffye's choice (1976-1979):** he adopts a modeling strategy based on the double fact that:
 - 1. Unlike the topologies of some algae (modeled through non parametric L-systems: 1968) or of some ferns (modeled through approximate Fractals: 1968), the topology of superior (vegetative) plants **can not be formalized through a unique overarching formalism**
 - 2. That this topology is nothing but **the topological result of the elementary and successive behaviors of all its burgeons**

I- 1st step : Pluriformalization of growing vegetative plants (6)

- The tree as a population of meristems

Three events are possible for a burgeon :

- 1) growth
- 2) pause
- 3) ramification

= i.e. **stochastic events** (probability) with **variable** parameters according to the localization of the bud in the tree & the order of ramification (**complex** Markov Chain)

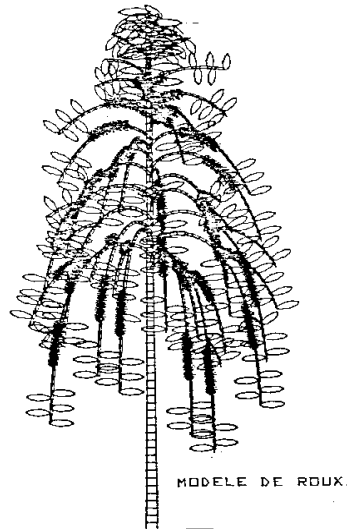
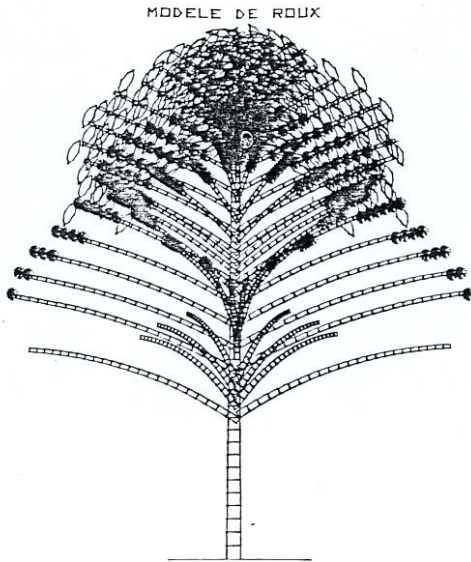
= Step by step reconstruction of the tree, replication of the global morphogenesis of the tree in a realistic manner

= **SIMULATION** (De Reffye - 1979)

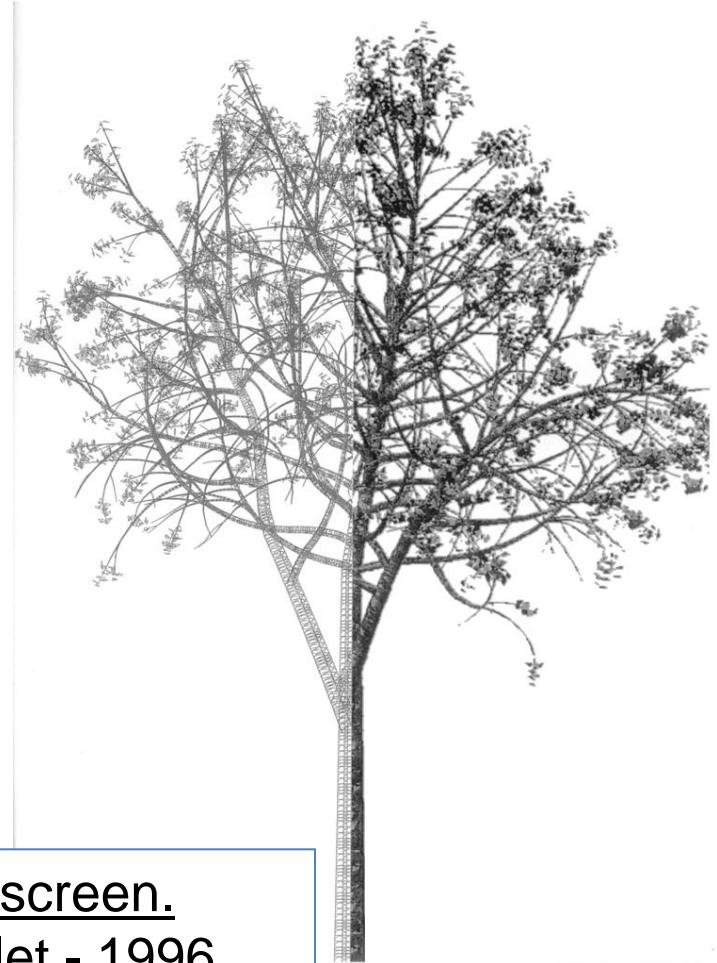


PLURIFORMALIZATION (not only discretization + probability)

- 1) fructification test : **topology** (ramification)
- 2) period of sunshine : **geometry** (related with the number of internodes that are present in the meristem and that really developed to form the growth unit)
- 3) breakage or folding of plants : **mechanics of axes** (physical laws of flexion due to the increase of masses of organs)



Coffee trees on plotter. Fructifer nodes (with cherries) and nodes with leaves. Topology, geometry and mechanics are taken into account (source: de Reffye's PhD, 1979)



Simulated tree (poplar) on bitmap screen.
Source : AMAP presentation booklet - 1996.

II- 2nd step: 4D simulations (1980-1998) (1)

- First software of AMAP (1985): AMAPsim (Jaeger's thesis – 1987):
 - Procedural programming
 - **Prefixed simulation**: all the order of ramification of a given branch of the tree (at a prefixed age) are completely simulated and developed, then the program goes to another branch, etc.
 - Simulation branch by branch: the **parallelism** of the working of burgeons is **not simulated**
 - **Mimetic in its result not in its trajectory** (epistemological outcome: simulation = not always a “model in time” nor “a process simulating another process” (Hartmann, 1996))

II- 2nd step: 4D simulations (1980-1998) (2)

- Second software of AMAP: AMAPpara (Blaise's thesis – 1991):
 - Object-oriented programming
 - Simulation of the parallelism of the burgeons
 - Biomimetic in its result and in its trajectory
 - Introduction of the notion of “physiological age” of burgeons (in order to automatize - with a biological meaning - the succession of the variable parameters of the statistical laws of ramification or pause, etc.)
 - Gives the possibility to add physiological submodels because of this mimetism in the trajectory: back to agronomy (the program can simulate the routes and the variable allocation of the products of photosynthesis at each moment of time)

II- 2nd step: 4D simulations (1980-1998) (3)

- **Limits of the simulation of parallelism (dynamical biomimetism)**
 - Integrating submodels of functioning (physiology) takes time and memory
 - Huge amount of computation steps (exponential increase)
 - Difficult to evaluate such many parameters even with data taken from the field: hence it is difficult to use AMAPpara as a normalized tool in agronomy
- **4 possible solutions:**
 - 1) A conciliation with some approaches using parametrized L-systems (Winfried Kurth, 1995), Prusinkiewicz school
 - 2) Try to invent some mathematical concepts which could help to directly uniformize such a pluriformalization (Godin, Caraglio, 1998): “A multi-scale model of plant topological structures”
 - 3) Simplify the program *ex post*
 - 4) Try to use some empirical laws that could help to make some short-cuts in this huge amount of computation steps

III- 3rd step: Remathematization of complex simulations (since 1998) (1)

- The last two solutions have been chosen by de Reffye: **simplifying the program, using empirical physiological laws** (e.g.: the phenomenological law of “water-efficiency”)
- But other solutions can work.
- Especially the number one: from this viewpoint, in my book (Varenne, 2007 ; 2018), through some analyses of quite recent publications I show the recent convergence between the school of Prusinkiewicz and de Reffye’s school

III- 3rd step: Remathematization of complex simulations (since 1998) (2)

- **Simplification of simulation through **structure factorization****

- 1998-2000: the team AMAP/LIAMA/INRIA observes that simulated trees can present more than 600 times the same sub-structure (= type of branch, metamer)
- Then, by observing the behavior of the program, it appears that it is not necessary to rebuild one by one all these metamers that are of the same type [\[1\]](#).
- A type of metamer is calculated once for all. The automaton commands its reiteration with a certain probability: and the resulting statistical architecture and physiological features of the simulated tree are almost exactly the same in terms of stochasticity and variability than the one of the totally simulated tree (i.e. burgeon by burgeon).[\[2\]](#).

- **It is always Monte-Carlo but it can be 4000 times quicker than the previous program of AMAPpara.**

- **⇒ Significantly, the team describes this simulation **more in term of model** : the **GreenLaB model**: a **Functional-Structural Model**.**

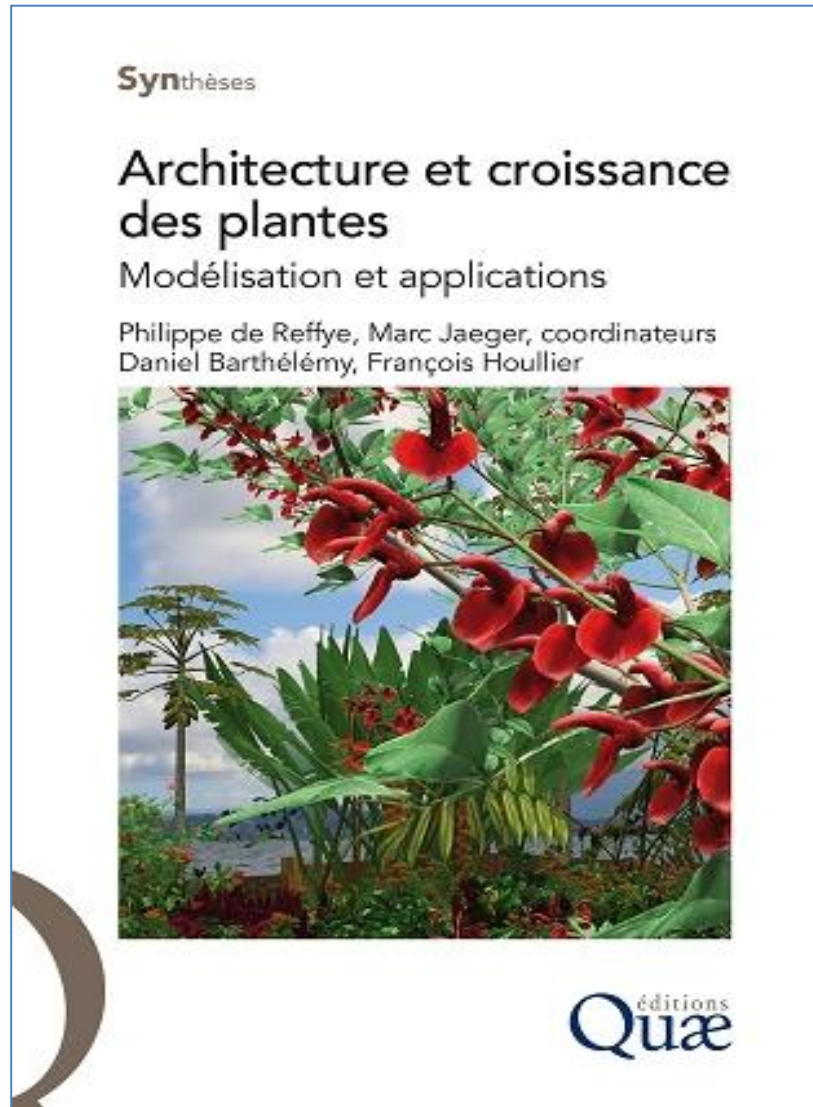
- [\[1\]](#) Reffye (de) (P.), Goursat (M.), Quadrat (J. P.), Hu (B. G.), « The dynamic equations of the tree morphogenesis GreenLab Model », dans B. G Hu., M. Jaeger (éd.), *Plant Growth Modeling and Applications*, Beijing, China, 2003, Hardcover, p. 109.
- [\[2\]](#) Cf. Kang (M. Z.), Reffye (de) (P.), Barczi (J. F.), Hu (B. G.), « Fast Algorithm for Stochastic Tree Computation », *Journal of WSCG (Winter School of Computer Graphics)*, 2003, vol. 11, n°1, p. 5.
- [\[4\]](#) Yan (H. P.), Reffye (de) (P.), Le Roux (J.), Hu (B. G.), « Study of Plant Growth Behaviors Simulated by the Functional-structural Plant Model GreenLab », dans B. G Hu., M. Jaeger (éd.), *op. cit.*, p. 118-122.
- Source: F. Varenne, 2007 & 2018, chap. 7.

III- 3rd step: Remathematization of complex simulations (since 1998) (3)

- **Algorithm analysis** and the return of formal (algebraic) calculus (INRIA)

- Not only the performance but also the structure of the program can be analyzed
- Fundamental ideas: optimization of algorithms for Multi-type branching process (T.E. Harris, 1963, chap. 15): **stochastic simulations can be remathematized** through **recurrent matrix equations** .
- See the recent works of P. H. Cournède, M. Z. Kang, A. Mathieu, P. de Reffye, B. G. Hu, J. F. Barczi, H.P. Yan, D. Auclair (2006-2010)
- **Return of analytical calculus** based on some key (because abbreviating) values: variance and mean of the number of organs, etc.
- From this evolution, it follows that spatialization and visualization are not so important as in the 4D simulation phase.
- There are a possible outcome of the calculus of the model but not a necessary means of computation.
 - Sources: Varenne 2007 & 2018 ; PH Cournède Habilitation's Thesis, 2009 (on line).

Most recent source



Architecture et croissance des plantes
– Modélisation et applications, de
Reffye et al., Paris, Quae, 2017.

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 - because it stabilizes the phenomenon,
 - it makes heterogeneous data and concepts match each other in a formal construct through a step-by-step conciliation of data-driven submodels and concept-driven ones
 - it allows virtual experimentations in domains where there were no simple experimentation
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- Just as integro-differential concepts were built: 1- to be tractable by hands and pencil and 2- to be adapted to the instruments of the 17th century mechanics and to the limited area of the measurable reproducible phenomena of this time.

PART II: TOWARD THE NOTION OF SIMULATION

II- Toward the notion of simulation (1/5)

Source: “Framework for M&S with Agents...”, Varenne, 2010

- Computer simulations depend on **formal models** (helps to solve, calculate, validate)
- A **formal model is** a formal construct possessing a kind of unity and formal homogeneity so as to satisfy a specific request : prediction, explanation, communication, decision, computability, etc.

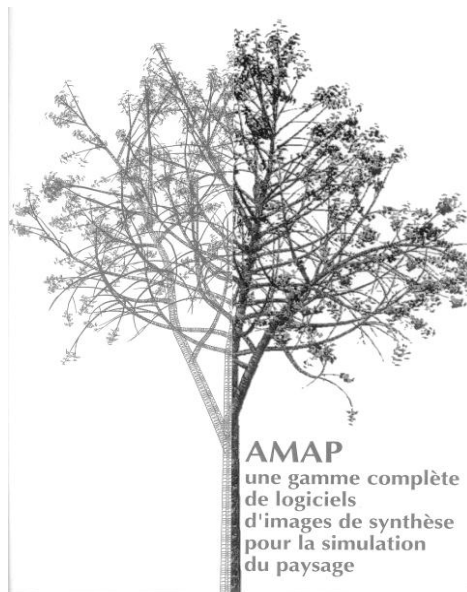
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- A **formal model** is a formal construct possessing a kind of unity and formal homogeneity so as to satisfy a specific request : prediction, explanation, communication, decision, computability, etc.
- Concerning **simulation**, current definitions need to be generalized.
- It is often said that “a simulation is a model in time”, a “**process that mimics the (supposed to be the more) relevant characteristics of a target process**”, Hartmann (1996). But consider:
 - The **variety** of types of contemporary CSs.
 - Today, CSs rarely are the dynamic evolution of **a single formal model**.
 - CSs in the sciences of complex objects are most of the time CSs of complex **systems of models**.
 - Moreover, there exist **various kinds of CSs** of the same model or of the same system of models.

II- Toward the notion of simulation (2/5)

- Last but not least, the **critereon of the “temporal mimicry”** is in crisis too: it is not always true that the dynamic aspect of the simulation imitates the temporal aspect of the target system. Some CSs can be said to be **mimetic in their results but non-mimetic in their trajectory** (Varenne, 2007) (Winsberg 2008).
- For instance, it is possible to simulate the growth of a botanical plant sequentially **and branch by branch** (through a non-mimetic trajectory) and not through a **realistic parallelism**, i.e. burgeon by burgeon (through a mimetic trajectory), and to obtain the same resulting and imitating image (Varenne 2007).



Source : Simulated Poplar - Plant
Architecture Modelling Laboratory
(CIRAD/France)

II- Toward the notion of simulation (3/5)

- The problem: the temporal aspect is itself dependent on the persistent - but vague - **notion of imitation or similitude**.
- But, in fact, it is possible to give a minimal characterization of a CS (not a definition) **referring neither to an absolute similitude (formal or material) nor to a dynamical model**.
- Let's say that **a simulation is a strategy of symbolization taking the form of at least one step by step treatment**. This step by step treatment proceeds in two major phases:
 - **1st phase (operational phase)**: a certain amount of operations **running on symbolic entities (taken as such)** which are supposed to denote either real or fictional entities, reified rules, etc.
 - **2nd phase (observational phase)**: an observation or a measure or any **mathematical or computational re-use** of the result of this amount of operations taken as given through a visualizing display or a statistical treatment or any kind of external or internal evaluations.
 - e.g., in some CSs, the simulated “data” are taken as genuine data for a model or another simulation, etc.

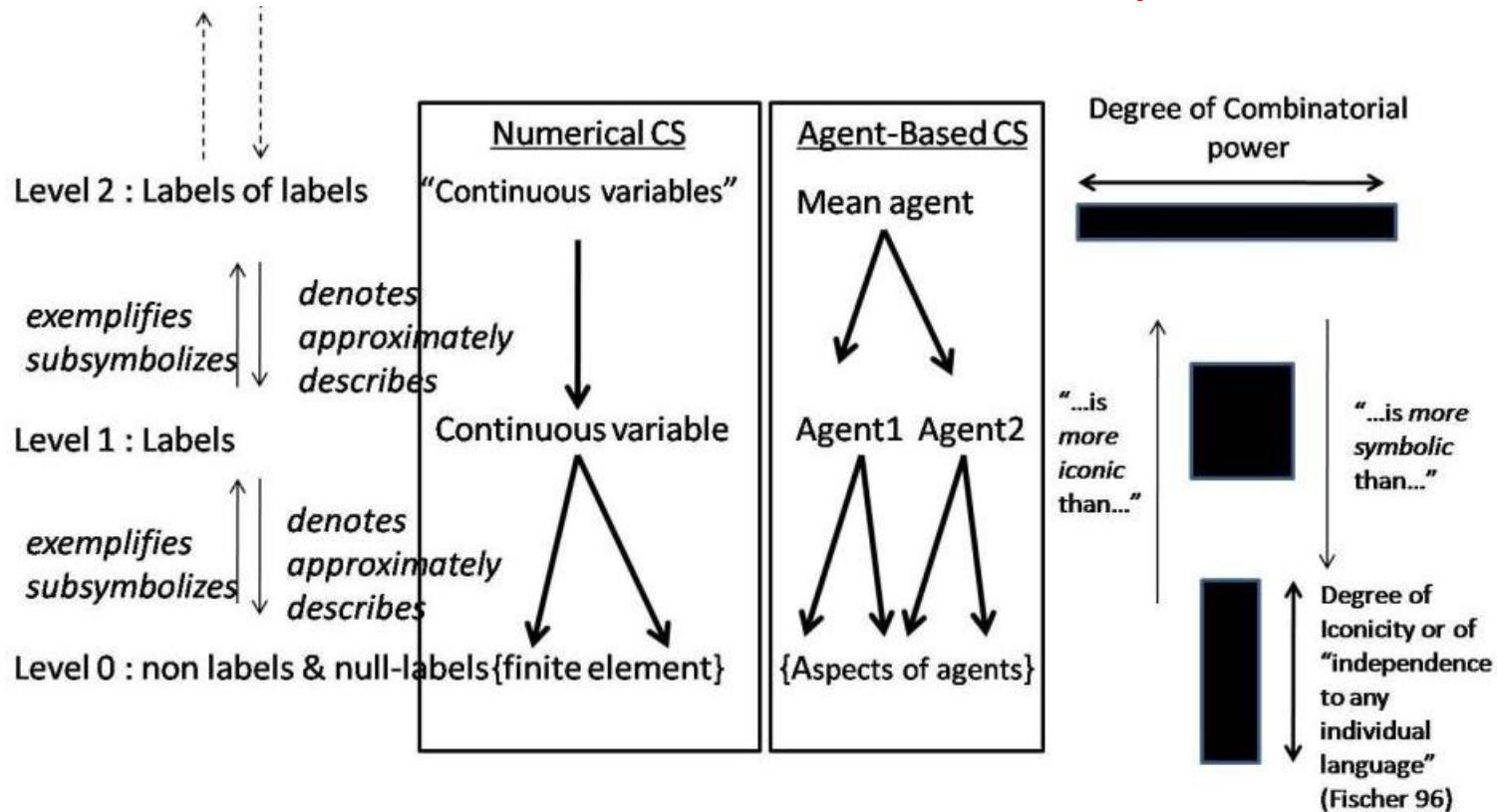
II- Toward the notion of Simulation (4/5)

Sub-symbolhood in computer simulations

- Concerning the two phases in simulation (operative, observational):
 - During the observational phase, **marks which were first treated as genuine symbols**, i.e. as denoting entities, are **finally treated as sub-symbols**: Why? They are **treated at another level** at the one they first operated.
 - At the end of process, it is the result observed - as a whole - which gains a proper and new symbolic nature
 - And this is relatively to this new symbol or system of symbols that the first symbols become sub-symbols.
 - Let's recall that, according to (Smolensky 1988), subsymbols operate in a connectionist network at a lower level than the symbols. As such, they can be seen as constituents of symbols.
 - Subsymbols “participate in numerical – not symbolic – computation”: the kinds of operation on symbols (computations) are not the same at each level.

II- Toward the notion of simulation (5/5)

Simulations and hierarchies of symbols

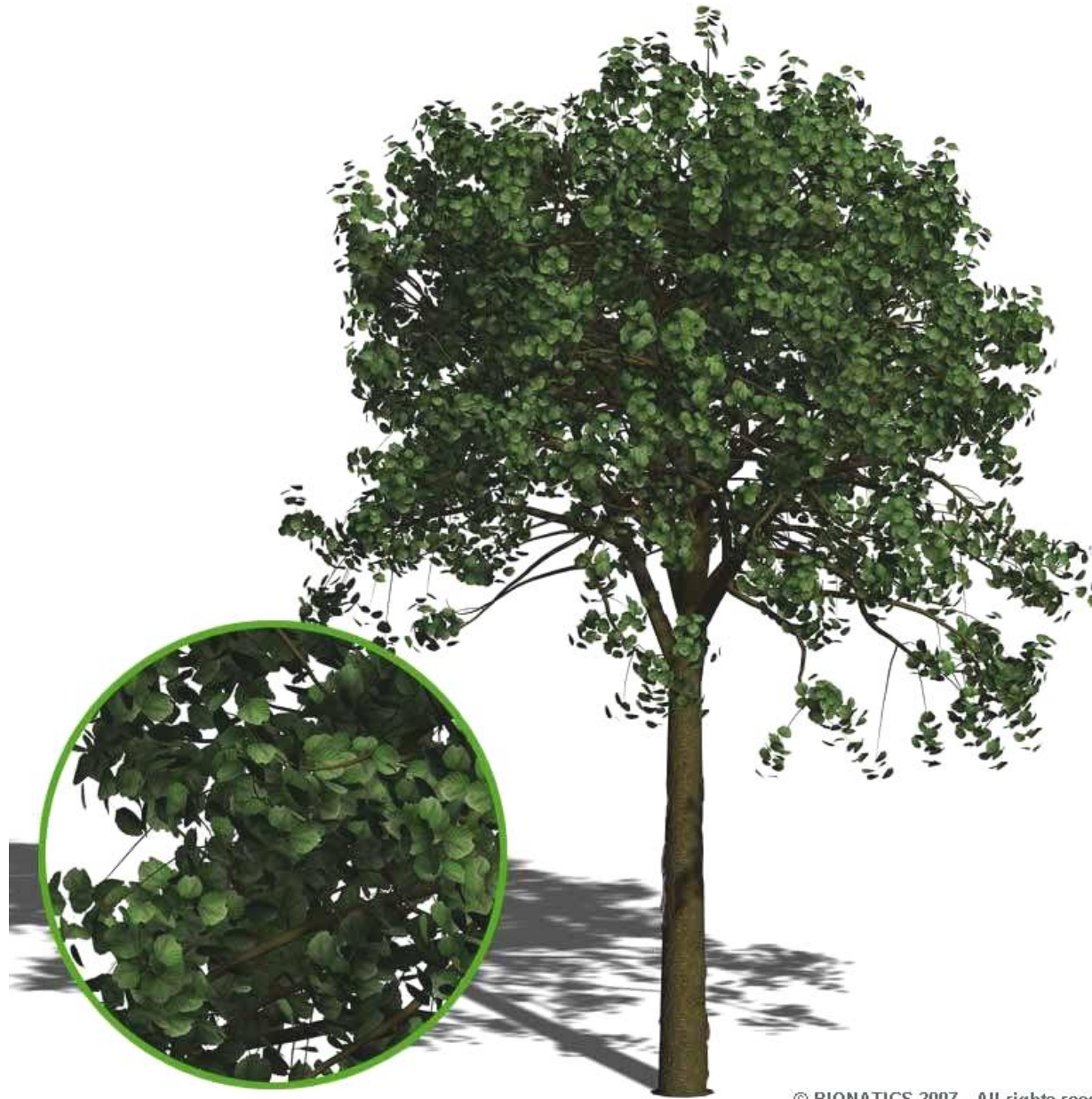


-We can draw a parallel between **the hierarchy of levels of symbols** in a symbols' hierarchy and the **similar hierarchies in numerical simulations and in agent-based simulations**.

-The relation of subsymbolization can be interpreted in terms of an **exemplification** whereas the relation of **denotation** can be interpreted in terms of an approximate description.

Part III- Examples of **integrative spatial simulations** in biology

And some remarks on their methodological and epistemological consequences



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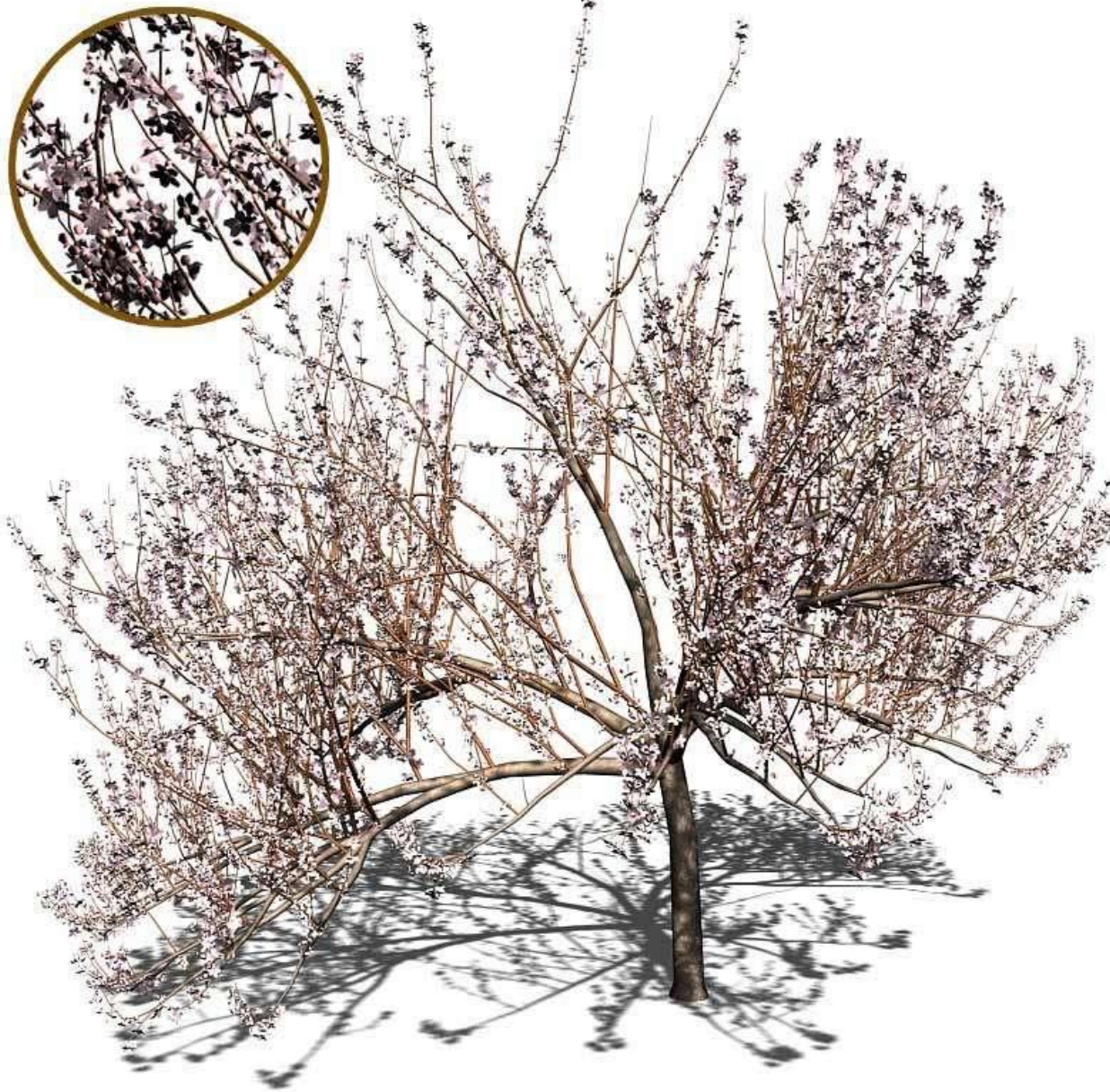
Alder - Source : Bionatics (<http://www.bionatics.com>)

Rapidly growing tree mature at about 60 years with long trunk and narrow crown. Distinctive outline in winter. Height 20m or more.



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Acacia Lahia - Source : Bionatics (<http://www.bionatics.com>)
A perennial flat-topped species of tree found in Africa.



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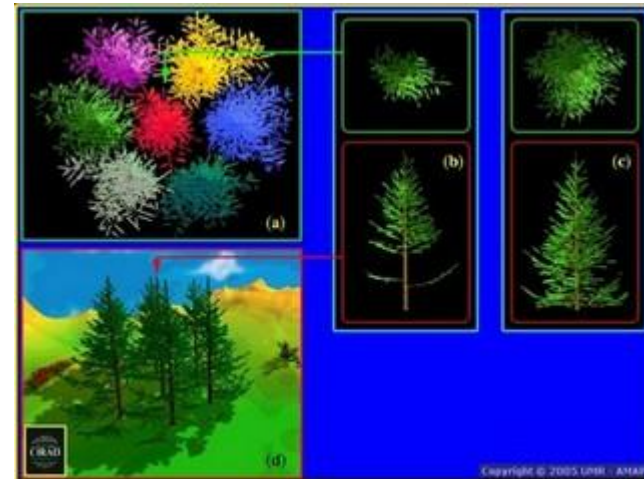
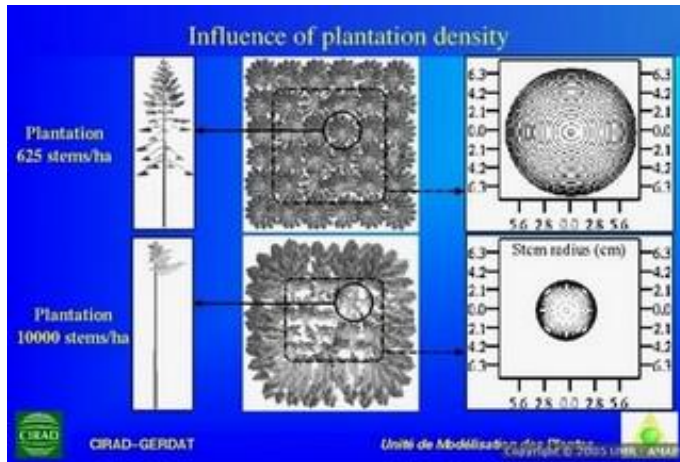
Japanese Apricot tree - Source : Bionatics (<http://www.bionatics.com>)
Low spreading tree with pink flowers in spring.

What for ?



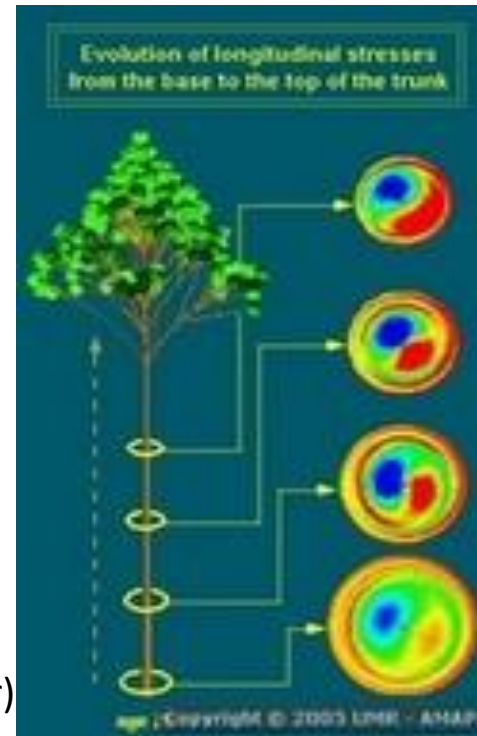
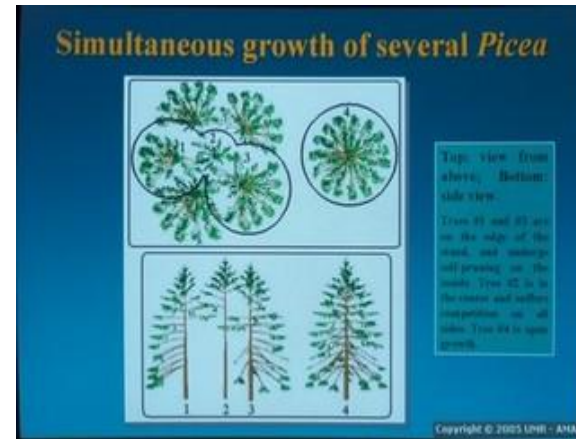
Copyright Alejandro Diaz - Architecture Visualized

Internal and External Interactions



Source: AMAP (CIRAD, INRIA, INRA, IRD, CNRS, Montpellier)

Interactions, flexions, mechanical constraints → prediction of wood quality

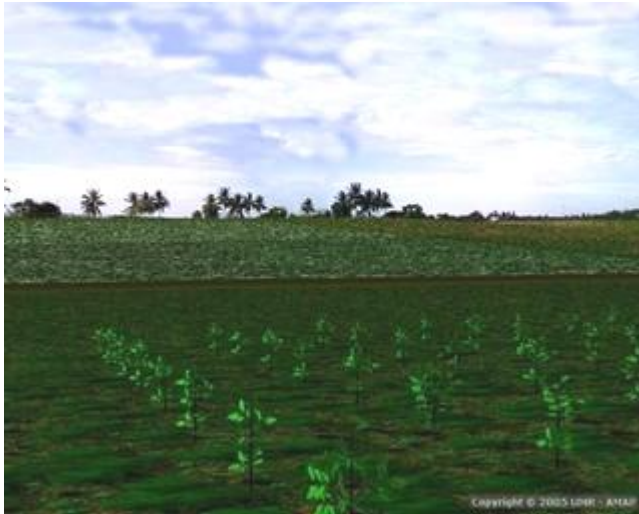


Applications in predictive agronomy : coffee, corn, ...



Source : Philippe de Reffye (Digiplante-Inria-ECP-INRA, Amap Cirad)

Applications in predictive agronomy



Virtual Coffee plantation

Source: AMAP (CIRAD, INRIA, INRA, IRD, CNRS, Montpellier)

Applications in urbanism...

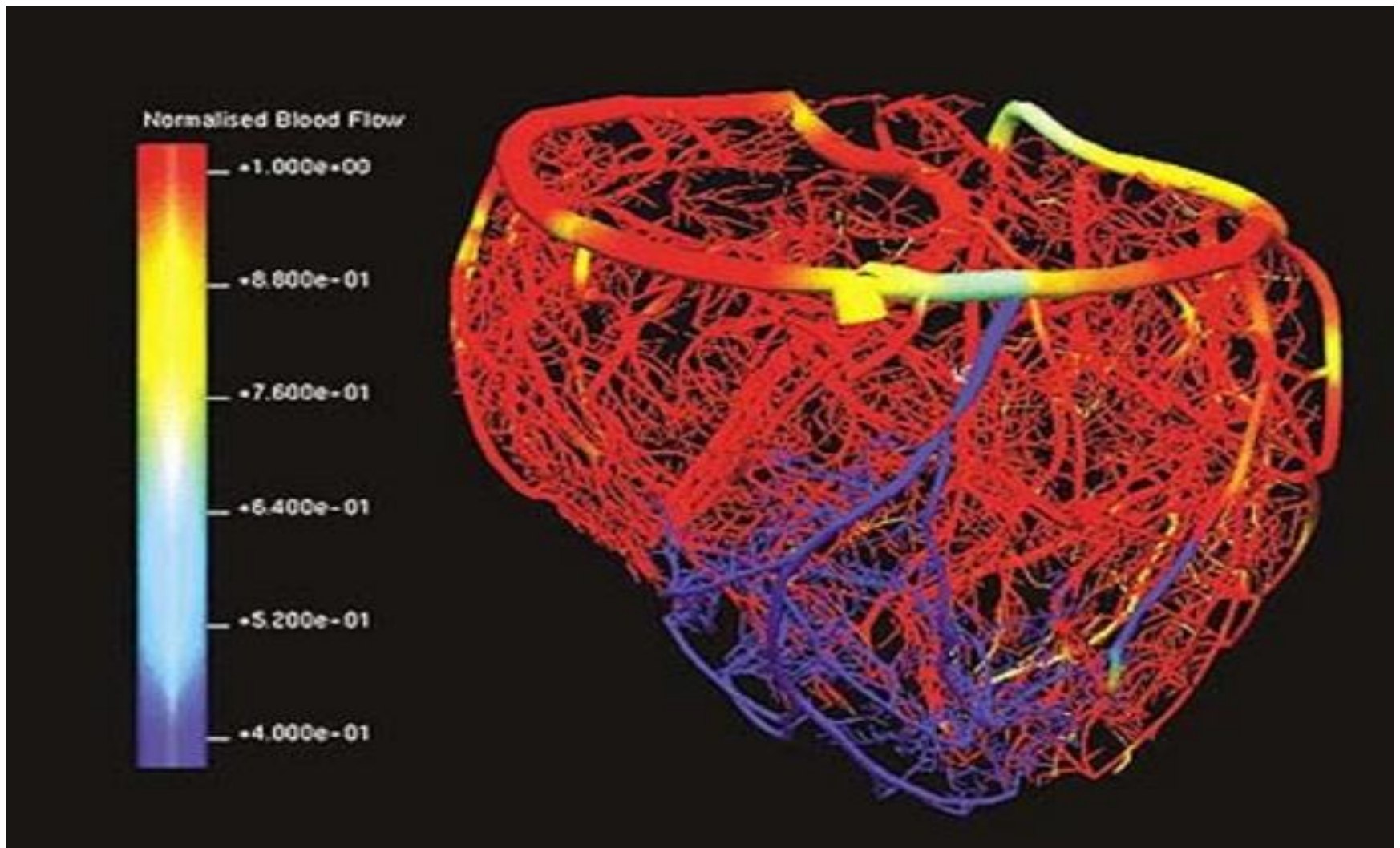


Source: AMAP (CIRAD, INRIA, INRA, IRD, CNRS, Montpellier)



Application in paysagism - Rehabilitation of an old quarry

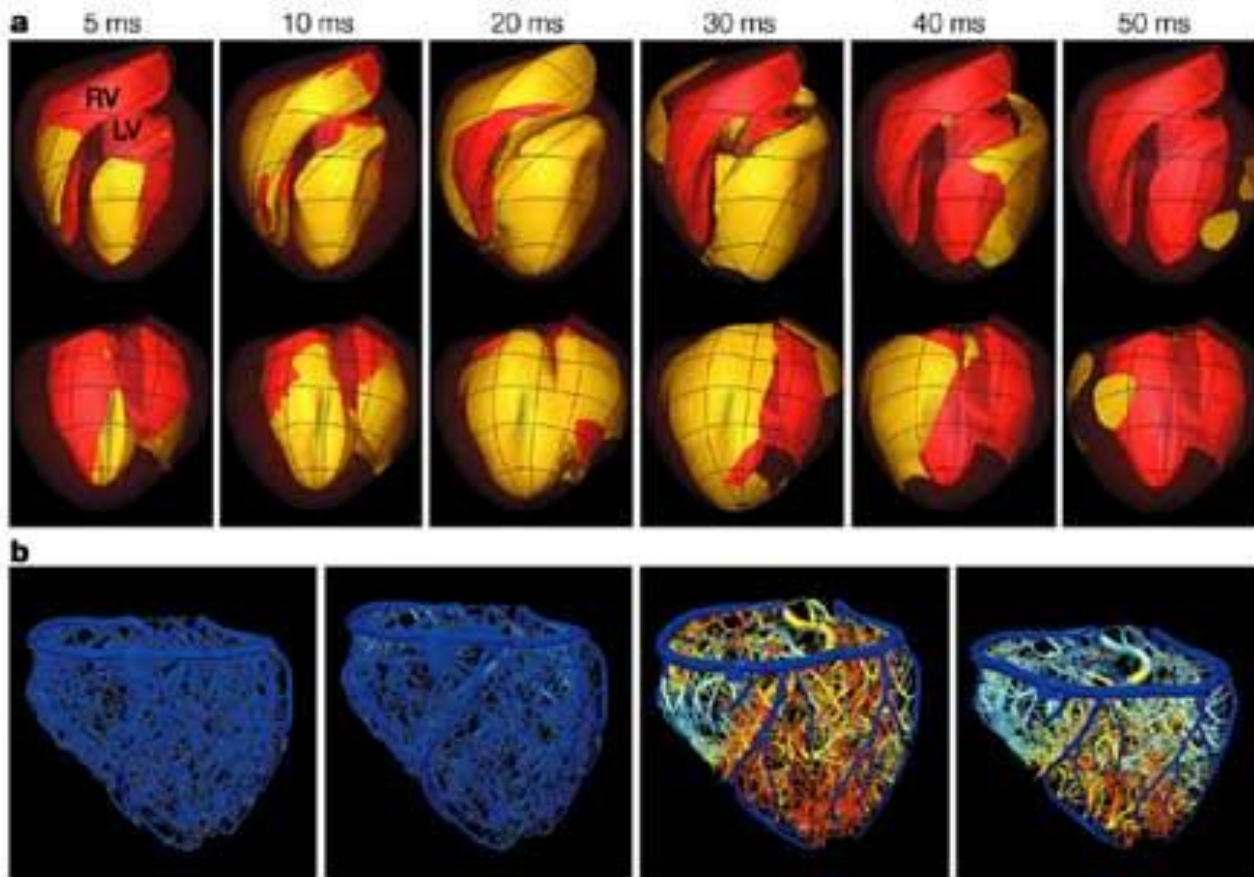
Source: AMAP (CIRAD, INRIA, INRA, IRD, CNRS, Montpellier)



Virtual heart - Denis Noble *et al.* (Oxford – Physiome Project)

*“The ‘Oxford Cardiac Electrophysiology Group’ led by Professor Denis Noble is an example for having developed a virtual model of the human heart, which **integrates** the kinetic characteristics of the **molecular** and **cellular** mechanisms of heart activity into **detailed anatomical** heart models and **allows forecasts** to be made on the **physiology and pathophysiology** of the heart”, Dr. Roland Eils (German Cancer Research).*

Source : <http://bio-pro.de/magazin/thema/00173/index.html?lang=en&artikelid=/artikel/03079/index.html>



Nature Reviews | Molecular Cell Biology

Physiome Project : Auckland, Oxford, San Diego

Source : http://www.nature.com/nrm/journal/v4/n3/box/nrm1054_BX2.html

The era of « Multis »

-1- Multi-aspectual

-2- Multiscale

- 3- Multi-physical : electrical, mechanical, chemical phenomena

- 4- Multidisciplinary: chemistry, mechanics, electricity, biology...

- 5- Multifield

Specifically, if an integrative simulation is not reducible to data-fusion (data-fusion = “action / decision oriented” integrative simulation for detection of targets or weapons), **this multiplicity implies too :**

- **Multi-scale**
- **Multiplicity of epistemic status** of the submodels of each scale or each aspect : (Varenne, 2007, 2008)
 - explanative submodels with verified or hypothesized mechanisms
 - phenomenological submodels (stochastic processes, Monte Carlo...)
 - digitalization of captured scenes
 - IRM scannings
 - ...
- **Inter-models explanation** : explanation through
 - “Emergence”
 - **or not** : only interactions at runtime between elementary mechanisms: “phenomenological reconstruction” [see (Peyrieras *et al.*) on the first steps of the ontogenesis of the zebra fish embryo: filiations cell by cell]

PART IV- ON SOME SPATIAL SIMULATIONS IN SOCIAL SCIENCE

The “complexity vector” F

Complexification of formalisms can go further thanks to computers

Source: Varenne, 2009

- From chaos studies, emerge three distinct **properties for a formalism**:
 - (1) it is a **notation (N)**
 - (2) it enables **symbolic combination and manipulation (C)**
 - (3) it leads to formalized **solutions (S)**

- For each, let’s introduce a **distinctive attribute**: “Simple”/”Complex”

- Vector F (for Formalism):

F (attribute of **Notation**, attribute of **Combination**, attribute of **Solution**)

- For instance, the claim about the formalism used by Poincaré can be represented by the complexity vector:

$F(S, S, C)$

Which means : the possibility of the Hamiltonian to always lead to a simple solution in the case of the 3-bodies problem is denied

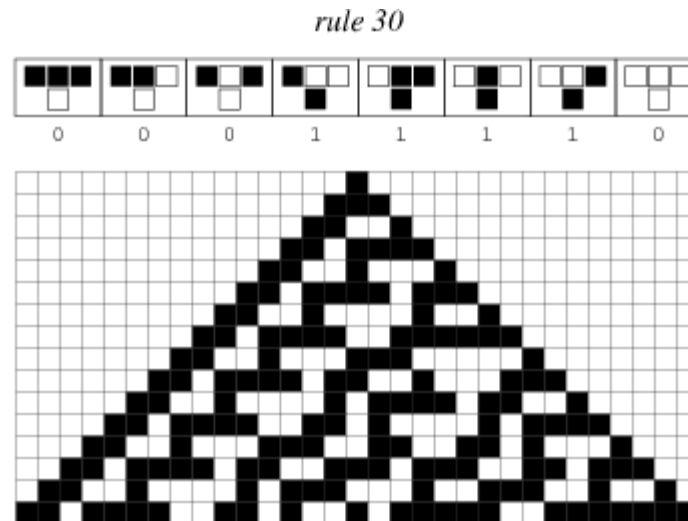
Complex Models of Complex Systems (1/3)

Cellular Automata

- *Complexification of formalisms can go further thanks to computers :*

F(S,S,C) (simple CA)
or **F(S,C,C)** (complex CA)

- *“A cellular automaton is a collection of ‘colored’ cells on a grid of specified shape that evolves through a number of **discrete time steps** according to a **set of rules** based on the states of neighboring cells. The rules are then **applied iteratively** for as many time steps as desired”* Source: Wolfram MathWorld. (Ulam, Metropolis and von Neumann)

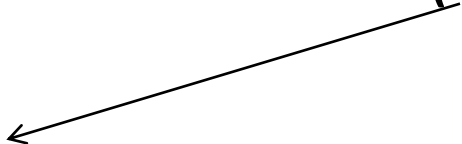


Complex Models of Complex Systems (2/3)

Multi-Agents Systems (MAS) of Complex Adaptive Systems (CAS)

- Complexification again: MAS after CA
- MAS according to Nigel Gilbert (2008):
 - Autonomy (like CAs: no general controller)
 - Social capacity (communication)
 - Reactivity (adapted to the environment)
 - Proactivity (purposeful: goal, values...)

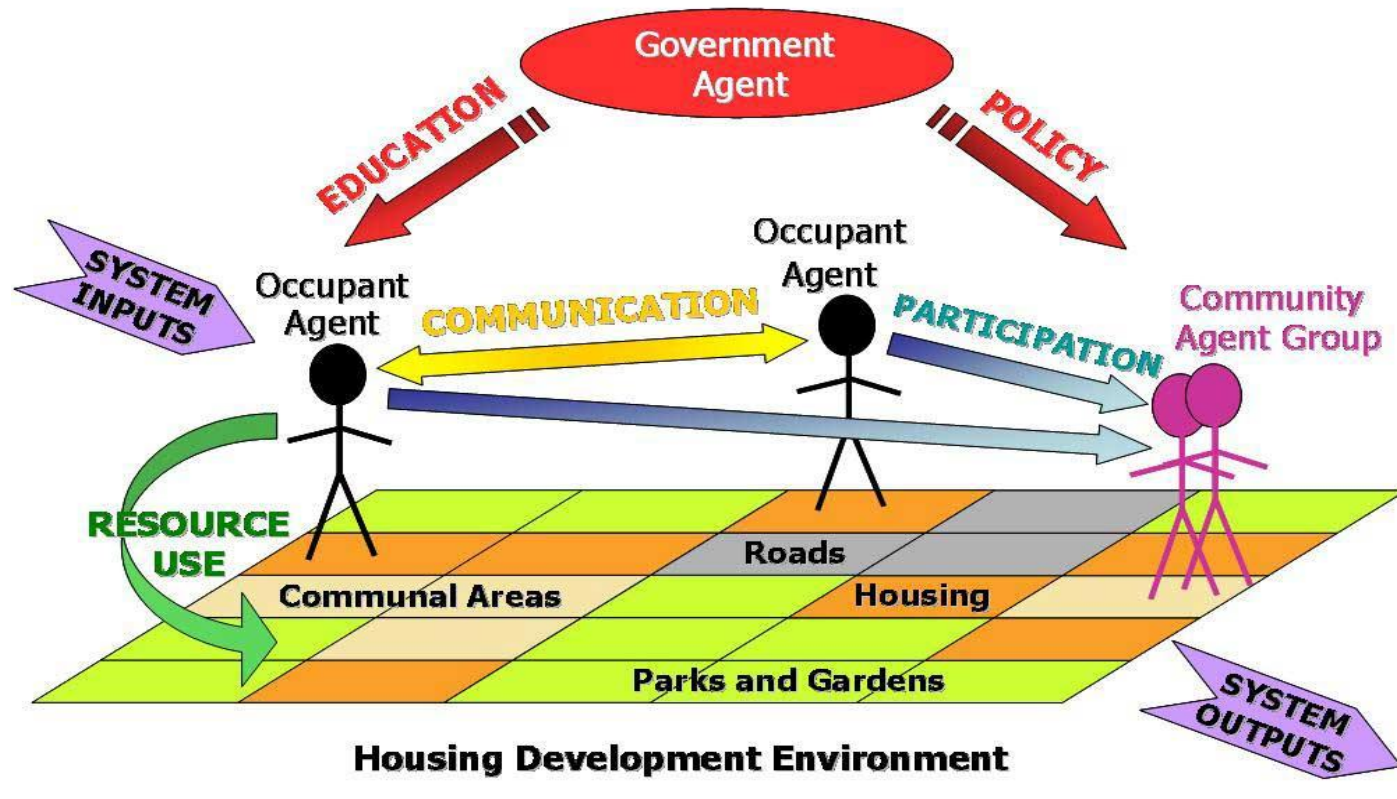
$F(C,C,C)$



- **Notation is being complexified: through software-based models of simulation**
- **Hence the necessity to standardize the notation process : e.g. the ODD protocol** (Overview, Design concepts, Details) of the Volker Grimm's team

Complex Models of Complex Systems (3/3)

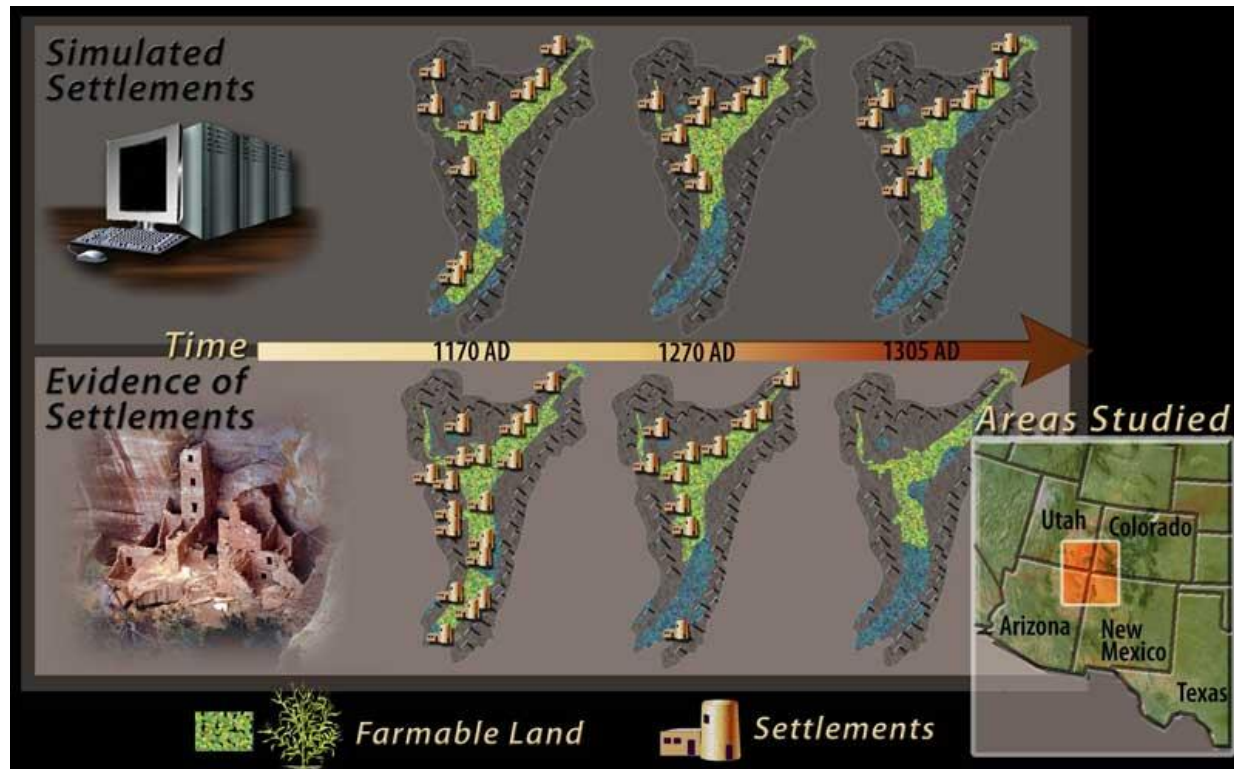
Multi-Agents Systems (MAS) - Example #1



“A multi-agent based model of the housing development that incorporates all of the resource models and the behavioural typology and interactions of the occupant agents”. Source : *Complex Science for a Complex World*, ANU, 2006, K.A Daniel, et al, p. 125 http://epress.anu.edu.au/cs/mobile_devices/index.html

Simulating Ancient Societies – MAS - Example #2

Virtual experimental archeology - Tim Kohler (Washington State University) & George Gumerman (School of American Research - Santa Fe)



The « Pueblo » people or Anasazi have lived during centuries in a south-west region of the USA
They suddenly abandoned the region in the 14th century (AD).

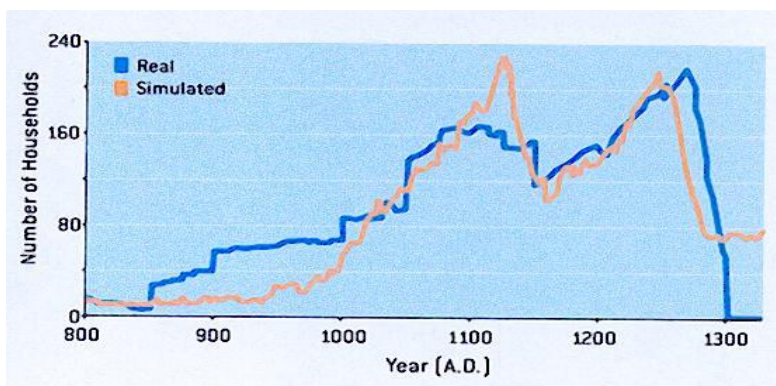
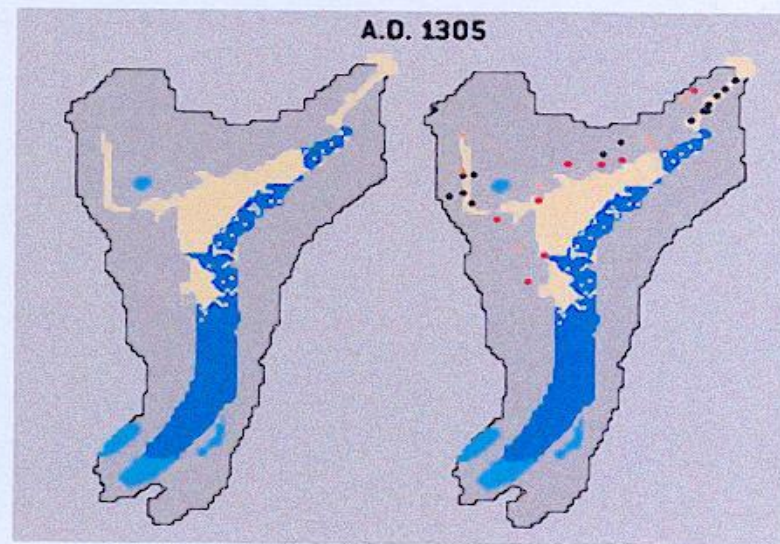
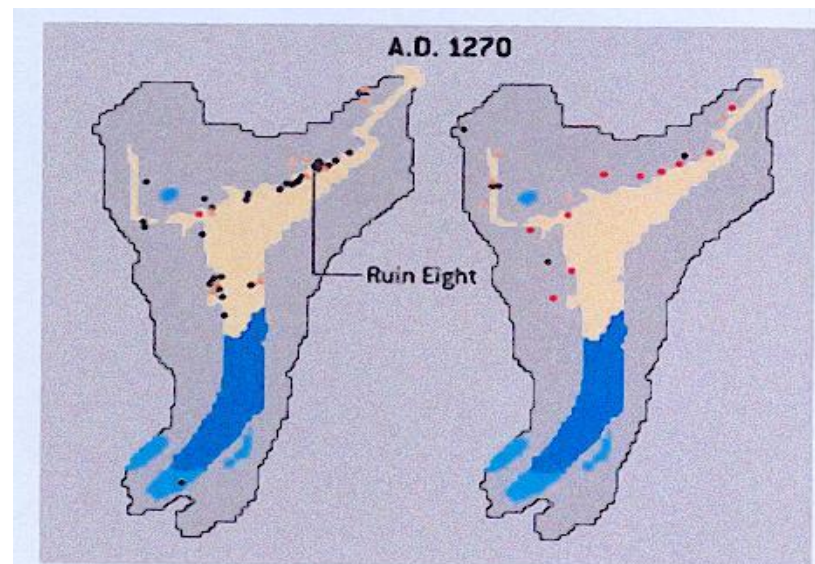
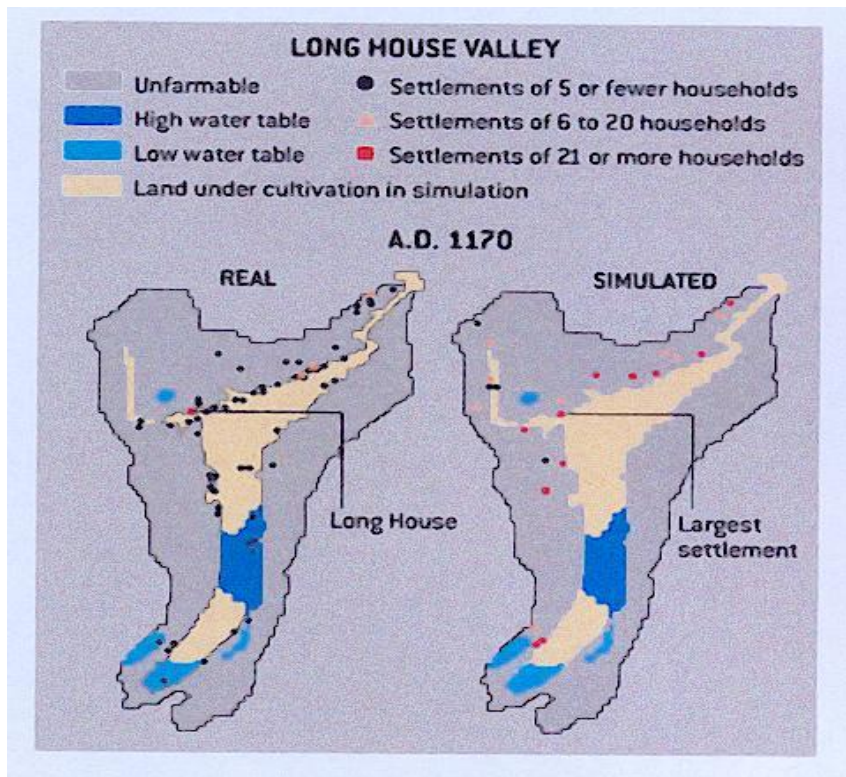
How to explain this?

Source : NSF - http://www.nsf.gov/news/news_summ.jsp?cntn_id=104261

Fundamental ideas of Kohler's simulations

- Agents are interacting and evolving
- They are evolving
 - 1) according to incorporated rules of behavior and
 - 2) according to their evolving environment (hence : MAS).
- We have diverse and dynamic environmental data
- Initial conditions: random distribution of the households
- The aim: observe on the simulation if it can predict (represent) the ulterior effective evolution (which has been recorded by the archeological data)

Results



Source : « Simulating Ancient Societies », *Scientific American*, 2005, Timothy A. Kohler, George J. Gumerman and Robert G. Reynolds

Some conclusions on the functions of spatial simulations

- New ways of representing, of imaging

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- New ways of experimenting: experimenting on interactions between symbols that have not always the same level of conventionality, hence the role of phenomenological reconstruction before any global theorization.
- New ways to experiment on emergence, on emerging patterns or to “program” emergence
 - With a problem : is a computational emergence a good representation/model of real biological or geographical emergence ? (Varenne 2012 “La reconstruction phénoménologique par simulation : vers une épaisseur du *simulat*” ; Varenne, 2013 : “Chains of Reference in Computer Simulations” ; Varenne, Cigenau, Petitot, Doursat, “Programming the emergence in MACS” *Acta Biotheoretica*”, 2015)

Thank you !