Simulation & Multi-Agent Systems
An Introduction
Digital Culture

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Next in Line...

Focus on. . .

Complex Systems? I

Several definitions—more ore less formal

- a complex system is a highly-structured system, which shows structure with variations
- a complex system is one whose evolution is very sensitive to initial conditions or to small perturbations, one in which the number of independent interacting components is large, or one in which there are multiple pathways by which the system can evolve
- a complex system is one that by design or function or both is difficult to understand and verify
- a complex system is one in which there are multiple interactions between many different components
- complex systems are systems in process that constantly evolve and unfold over time

Complex Systems? II

emergent phenomena which result from the interactions of individual autonomous entities

$\downarrow$

"the whole is more then the sum of its parts"

Features of Complex Systems in a Nutshell

- research on complex systems is (still) a hot topic for both scientists and engineers
- common features of complex systems of any sort include
  - *nonlinear* dynamics
  - presence of positive and negative *feedbacks*
  - ability of *evolution* and *adaptation*
  - *robustness*
  - *self-organisation*
  - *hierarchical* organisation
  - autonomy
  - ! their internal structure and inter-component interaction are typically studied via simulation

A Step Backward: The Scientific Method

Traditional science workflow [Parisi, 2001]

- identification of the *phenomena* of interest
- direct *observation* of the phenomena
- formulation of theories / working *hypothesis*
- *reasoning* on theories and phenomena through an empirical observation
- quantitative analysis: *measuring* of phenomena in laboratory under controlled conditions
- *validation* / *refutation* of theories

Issues

What if. . . [Parisi, 2001, Klugl and Norling, 2006]

- the system cannot actually be *observed*
  - for either ethical or practical reasons
- the *time scale* of the real system is either too small or too large for observation
- the original system is *not existing* anymore or not yet
- the system is *complex*
  - simple pattern of repeated individual action can lead to extremely complex overall behaviour
  - it is – at least practically – impossible to predict a-priori the evolution of the system

What Can We Do for. . . [Parisi, 2001]

- making predictions to be tested by experiments
- exploring *questions* that are not amenable to experimental inquiry
- obtaining a better *understanding* of some features of the system
  - verifying hypothesis and theories underlying the model that try to explain the systems behaviour
- asking *"what if"* questions about the real system
  - analysing the effects of manipulating experimental conditions without having to perform complex experiments

Focus on. . .

Definition of Simulation

Simulation

- is introduced as a new way for describing scientific theories
- is defined as
  - the process with which we can study the *dynamic evolution* of a model system, usually through computational tools [Parisi, 2001]
  - the imitation of the operation of a real-world process or system over time [Banks, 1999]

Simulation Requires a Model I

Models, objects, observers, questions [Minsky, 1965]

To an observer B, an object A* is a model of an object A to the extent that B can use A* to answer questions that interest him about A.

Reformulation: models, systems, experiments [Röhl and Uhrmacher, 2005]

A model (M) for a system (S), and an experiment (E) is anything to which E can be applied in order to answer questions about S

Simulation Requires a Model II

- a *model* is a representation / abstraction of an actual *system*
- in terms of representation, a model is a formalisation of aspects of a real process that aims at precisely and usefully describing that process itself
- in terms of abstraction, the construction of a model typically involves aggregation, simplification, and omission
- the model implements *theories* that have to be verified during the simulation

Typical questions in model construction

- how complex should be the model?
- which assumptions should be made?

From Model to Simulation. . .

Computer simulation

- computer simulation represents a way to exploit a computational model
- models are designed to be run *as processes* within a computer
- simulation creates a virtual laboratory, where
  - *virtual phenomena* can be observed under controlled conditions
  - the components of an experiment (variables, parameters, . . .) can be easily *modified*
- sequences of simulations can imitate operations of the modelled process
  - enabling the generation of an artificial evolution of the system

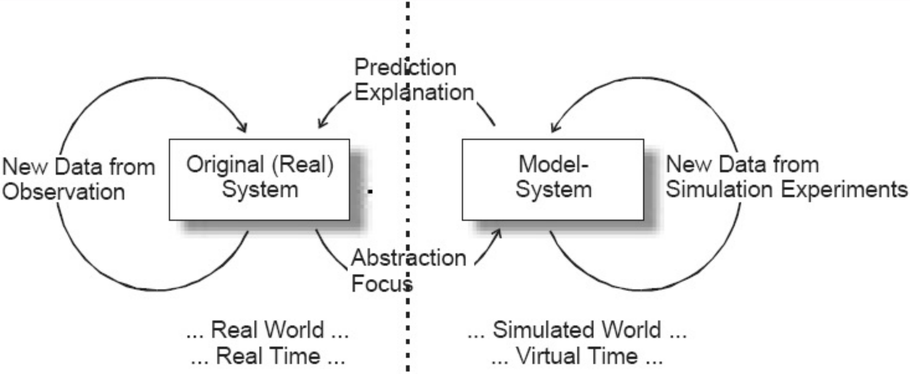
. . . and Back I

- the observation of the simulation carries out *deductions* on the *actual dynamics* of the real system represented
- simulation results make it possible to *evaluate theories* which the model is based on

. . . and Back II

Model validation [Klugl and Norling, 2006]

- if the *predicted* and *observed* behaviour do not match, and the *experimental data* is considered reliable, the model must be revised



Focus on. . .

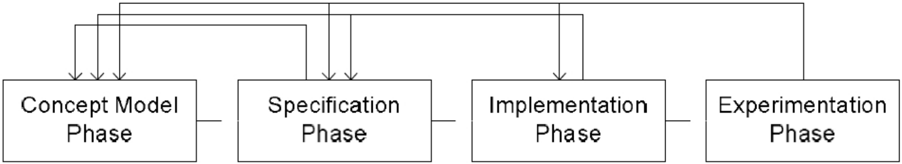
Simulation Workflow

Steps in a simulation study at a glance [Klugl and Norling, 2006]

- starting with a real system analysis
  - understanding its characteristics
- building a model from the real system
  - retaining aspects relevant to simulation
  - discarding aspects irrelevant to simulation
- constructing an executable representation of the model that can be run on a computer
- analysing simulation outputs, matching them against *real* system data
  - model validation and verification

How to Build a Model: Methodology I

Model design



How to Build a Model: Methodology II

domain model concept model phase

- analysis of the features of the real system

design model specification phase

- translation of the information collected in the domain model into a formal model

aim build a model (mostly) independent of any simulation tool or platform

computational model implementation phase

- translation of the design model resulting from the design on a particular software platform

Focus on...

Applications of Simulation I

A multi-disciplinary research field

Maths, physics, informatics, biology, economy, philosophy, medicine & health . . .

- complex dynamical systems
  - biological systems (e.g., brain, biomolecular/cellular biology)
  - clinical healthcare
  - social systems
  - ecosystems
  - economic systems
  - coordinating systems (e.g., swarm, flocking)
  - . . .

Applications of Simulation II

$\rightarrow$ systems too complex to be understood from observations and experiments alone

$\rightarrow$ systems that does not exist and, for instance, has to be built (*system engineering*)

Applications of Simulation III

Examples

- EU-FP7-FET Proactive project SAPERE Self-aware Pervasive Service Ecosystems, under contract no.256873
  - to construct an infrastructure for pervasive systems, e.g. steering users into complex environment, such as a city, avoiding obstacles (crowded areas, future street closure...)
- the black hole visualisation in Christopher Nolan's Interstellar
- H2020 calls for proposals

  PHC-28-2015 self management of health and disease and decision support systems based on predictive computer modelling used by the patient him or herself

  SC1-PM-17-2017 personalised computer models and in-silico systems for well-being

Autonomy & Simulation

What do all the above sorts of systems have in common?

- they *all* deal with systems exhibiting some sorts of *autonomous activity*
- either generated by the components / actors / agents
- or, by the environment
- or, again, by their structure / organisation / dynamics

Which sorts of computational systems should we use to simulate them?

- *multiagent* systems (MAS)
- *coordinated* systems

→ that is, those systems that can bring about *autonomy* via either *component behaviour* or *intra-system interaction*, respectively

Next in Line. . .

Granularity of Simulation Elements

Types of simulation [Uhrmacher et al., 2005]

Depending on the granularity of their simulation elements, simulation can be

- micro-level
- macro-level
- multi-level

Macro-simulation

Macro-simulation [Uhrmacher et al., 2005]

- the macro model describes the system *as one entity*
- the model attempts to simulate changes in the averaged characteristics of the whole population
- variables and their interdependencies, which can be expressed as rules, equations, constraints... are attributed to that entity
- modelling, simulating, and observation happens on one level: the *global level*
- the characteristics of a population are averaged altogether

Micro-simulation

Micro-simulation [Uhrmacher et al., 2005]

- the micro model describes the system *as a set of entities*
  - smaller entities with distinct state and behaviour
  - the system is conceived as including a numbers of entities
  - the system entities interact with each other
- the micro level models the behaviour of the individuals
- the macro level
  - exists only as it *aggregates* results of the *activities* at micro level
  - is used to express *emergent phenomena*

Multi-level Simulation

- it is an intermediate form
- the multi-level model describes a system at least at two different levels
- interactions are taking place *within* and *between* the different levels—both *intra-* and *inter-level*
- the system is described at *different time scales*

Benefits of multi-level simulation

- it makes it easier taking spatial and temporal structured processes into consideration
- it models the complex systems hierarchical organisation
- it allows the description of upward and downward *causation*

Downward and Upward Causation

F. Heylighen http://pespmc1.vub.ac.be/DOWNCAUS.html

The whole is to some degree constrained by the parts (upward causation), but at the same time the parts are to some degree constrained by the whole (downward causation).

How to Choose between Different Approaches

Which kind of simulation?

- modelling and simulating approaches are chosen on demand, thus they address the diverse, specific modelling and simulation needs of the given systems
- multi-level simulation is widely considered the most suitable approach for studying complex systems

Next in Line. . .

Differential Equations I

- system described by a set of *state variables*
- different types of differential equations

  Ordinary Differential Equations (ODE) — specifying how do variables vary in time

  Partial Differential Equations (PDE) — specifying how do variables vary in time and space

  Stochastic Differential Equations (SDE) — specifying which is the probability associated to the (stochastic) variable
- time-dependent variables are assigned to different measurable or not-measurable quantities of the system
- the continuous state changes are modelled by a sum of rates describing the increase and decrease of quantities amounts.

Differential Equations II

Features

- continuous model
- deterministic vs. stochastic model
- macro model

An example of ODE

- the state variable is referenced as X_i which is a macroscopic collective variable
- the collection of values of all these state variables $\{X_1, X_2, ..., X_n\}$ denote a complete set of variables to define the *instantaneous state* of the system $\mathbf{X}$
- the time evolution of $X_i(t)$ will take the following form, through a mathematical expression (ODE)

$$\frac{dX_i}{dt} = F_i(X_1, X_2, ..., X_n; \gamma_1, \gamma_2, ..., \gamma_m)$$

- where
  - F_i may be a complex function of the state variables: the structure of the function F_i will depend in a very specific way on the system considered
  - $\gamma_1, \gamma_2, ..., \gamma_m$, are the parameters of the problem (*control parameters*)

Simulation of Differential Equations Models I

Analytical solution of differential equations

- the exact solution of a class of differential equations is typically possible under very special circumstances
  - i.e. when the function F_i is linear
- example of analytic solution
  - the solution of a set of ODEs in terms of exponential functions, $\exp(\lambda_i t)$, and harmonic functions, $\sin(\omega_i t + \phi_i)$

Simulation of Differential Equations Models II

Numerical solution of differential equations

- also called *numerical integration*
- the exact solution of the equations is approximated by calculating approximate values $\{X_1, X_2, ..., X_n\}$ for $\mathbf{X}$
- time step is reduced to arbitrary small discrete intervals: values at consecutive time-points $t_0, t_1, ..., t_m$
- it uses different numerical algorithms
  - Euler's method for ODEs
  - Taylor series method for ODEs
  - Runge-Kutta method
  - Runge-Kutta-Fehlberg method
  - Adams-Bashforth-Moulton method
  - Finite Difference method for PDEs
  - ...

Simulation of Differential Equations Models III

Qualitative solution of differential equations

- it answer qualitative questions such as
  - what will the system do for $t \to \infty$
  - under which condition the system is *stable*
- definition of system attractors
  - equilibrium points
  - limit cycles
  - strange attractors
- bifurcation analysis
  - how the system's dynamic (solution) changes under the change of its parameters

Modelling a Complex System

Recap

- important features of a complex systems
  - systems that draw their dynamics from flexible local interactions
  - systems where individuality and/or locality is important
  - systems with a strong hierarchical organisation
  - emergent phenomena and self-organising systems
  - downward and upward systems dynamics
- essential to model a complex system
- relevant for analysing and choosing modelling approaches and tools

Analysis of Differential Equations I

Advantages of ODE and PDE

- they are a really *well-understood* and well-established framework
- they are relatively *simple*
- they have a strong *formal* aspect

- where do differential equations *fail*?

Analysis of Differential Equations II

Are *DE they able to capture features of complex systems?

Top-down approaches—macro model

- the model is built upon the imposition of *global laws*
- the model *loses* the representation of the *actors* of the system
- focussing only on the population, the model *loses* the representation of the *individual* and of its *locality*
- the model does *not* allow the study of global dynamics as *emergent phenomena* from local interaction
- the model *ignores* the *local processes* performed by low-level components
- a *particular entity* is no longer accessible

Next in Line. . .

Why do We Need Agent-Based Models (ABM)?

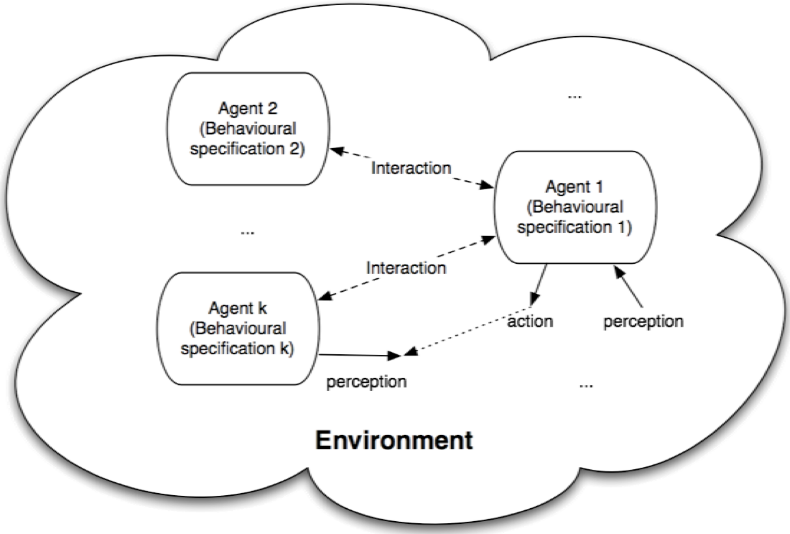
- several situations are characterised by the presence of autonomous entities whose actions and interactions determine (in a non-trivial way) the evolution of the system
- a growing number of disciplines are interested in studying effects of
  - local-global interaction, self-organisation, emergence, heterogeneity

Agent-based models (ABM) are particularly suited to represent such sorts of situations, and to support this kind of study and analysis

ABM make it possible to. . .

1. model the *individual properties* that cannot be fully taken into account by the state variables of the model
2. understand how *individual* properties determine *system-level* properties
3. capture the *hierarchical organisation* of complex systems
4. explore the role of the *environment*

ABM in a Picture [Vizzari, 2009]



What are ABM? I

Definition

An agent-based model (ABM) is a specific individual-based computational model for studying macro emergent phenomena through the definition of the system micro level which is modelled as a collection of interacting entities.

What are ABM? II

- MAS provides designers and developers with...

  agents — ... a way of structuring a model around *autonomous*, heterogeneous, communicative, possibly adaptive, intelligent, mobile, ... entities

  society — ... a way of representing a group of entities whose behaviour emerges from the interaction among element

  environment — ... a way of modelling an environment characterised by a topology and complex internal dynamics

- MAS gives methods to...
  - model individual structures and behaviours of different entities
  - model local interactions among entities and entities-environment
  - model the environment structures and dynamics

What is Multi-agent Based Simulation (MABS)?

Executing an ABM for a simulation amounts at

- running an ABM
  - computational engine for simulating agent behaviours and interactions
- studying its evolution
  - observing individual and environment evolution
  - observing global system properties as emergent properties from the system's constituent units interactions (from the bottom-up)
  - making *in-silico* experiment
- an agent-based modelling toolkit and a programming language is needed

When to Use ABM?

- when there are decisions and behaviours that can be defined discretely (with boundaries)
- when the individual behaviour
  - is non-linear
  - can be characterised by thresholds or if-then rules
  - exhibits memory and path-dependence or even adaptation and learning capabilities
- when interactions with flexible individual participants have to be represented
- when in-homogeneous space is relevant
- when the topology of the interactions is heterogeneous, and cannot be abstracted away
- when the system consists in mutable interacting participants (*openness*)
  - agents can leave, and new agents can enter the scenario
- when averages will not work / will not tell us what we need

Benefits and Drawbacks of ABM I

Benefits

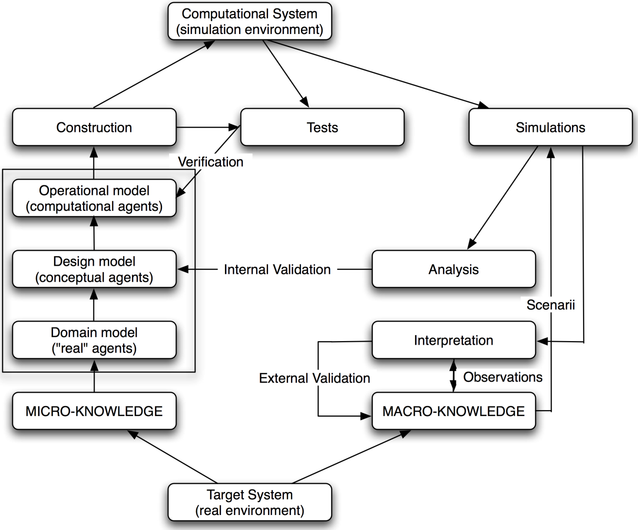
- it provides a straightforward description of a system
- → it makes the model look closer to the system, when observed
- it is flexible
- it captures emergent phenomena

Benefits and Drawbacks of ABM II

Drawbacks

- there is a lack of
  - an unified formal framework for unambiguously representing ABM elements and rules
  - a widely accepted methodology for developing MABS
- it increases the number of parameters
- software development remains a significant barrier to the use of ABM
  - typically leading to unintended incongruence between agents of the conceptual model and agents of the computational model

The Methodology in a Picture



Defining Agents of an ABM I

The keys for developing useful ABM are

- identifying the agents
- accurately specifying their behaviours
- appropriately representing agent interactions

Defining Agents of an ABM II

An agent in ABM requires mechanisms for. . .

- receiving the input *e.g.*, through sensors
- storing history, *e.g.*, through a state
- autonomously devising their course of actions, *e.g.*, through decision rules defining their

  reactive behaviour — how an agent reacts to external stimuli without external direction

  proactive behaviour — how an agent behaves in order to reach its goals/tasks
- carrying out the action *e.g.*, through effectors

Agents might also have capability of *learning*

$\rightarrow$ processing the ability of adapting to changing environment

Multi-Agent Based Simulation Platforms I

Definition

MABS platforms are agent-based toolkits providing frameworks and libraries that simplify the procedures of establishing models and performing simulations

Multi-Agent Based Simulation Platforms II

Standard issues [Railsback et al., 2006]

- structure of the model—i.e., agent behaviour, agent communication mechanisms, environment and topology
- discrete-event simulation (DES)
  - scheduling — controlling which specific actions are executed and when (in simulated time)—time-stepped, activity-based, discrete-event simulation
  - Marsenne Twister — random number generation
- distributed simulation
- facilities for storing and displaying the simulation state

Most of the agent-based simulation platforms are based on the *object-oriented paradigm*

NetLogo `http://ccl.northwestern.edu/netlogo/`

The Logo family of platforms has followed a different evolution

- objectives
  - to be ease of use
- educational tool
- NetLogo is recommended for models
  - with short-term, local, interactions of agents
  - base on grid environment
  - not extremely complex
- useful for prototyping models (quickly) and exploring design decisions
- provided by an own programming language
  - high level structures and primitives
  - all code in the same file

Coherence between design and computational model still missing

Repast Simphony

Repast http://repast.sourceforge.net/

- Repast is free and open source
- an optional point-and-click model development environment that generates Java classes
- a point-and-click model execution environment that includes
  - built-in results logging
  - graphing tools
  - automated connections to a variety of external tools
- a flexible definition of space for modelling / visualising 2D / 3D environments
- a fully-concurrent multithreaded discrete event scheduler
- libraries for genetic algorithms, neural networks, regression, random number generation, and specialised mathematics
- automated Monte Carlo simulation framework

Many Other MABS Platforms

- Swarm
- MASON
- AnyLogic
- GAMA
- SugarScape
- ...

Applications of ABM

Enormous range of applications

1. modelling agent behaviour in the stock market
2. understanding consumer purchasing behaviour
3. modelling the adaptive immune system
4. predicting the spread of epidemics
5. understanding the fall of ancient civilisations
6. modelling the engagement of forces on the battlefield
7. analysing the behaviour of crowds of pedestrians
8. military planning
9. economics
10. ...

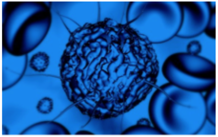
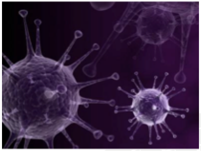
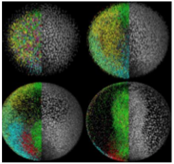
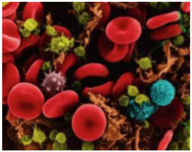
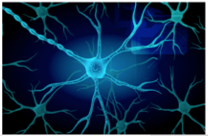
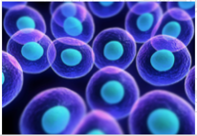
Next in Line. . .

Focus on. . .

Multicellular Systems

Multicellular systems are living organisms that are composed of numerous interacting cells. . . [1]

- immune system
- neural system
- embryogenesis
- adult stem cells
- tumor growth
- ...

On the Morphogenesis of Living Systems I

Developmental biology researches the mechanisms of development, differentiation, and growth in animals and plants at the molecular, cellular, and genetic levels.

Animal developmental steps

1. fertilisation of one egg
2. mitotic division
3. cellular differentiation
   - diverse gene expression
4. morphogenesis
   - control of the organised spatial distribution of the cell diversity

On the Morphogenesis of Living Systems II

Each region of the developing organism expresses a given set of genes

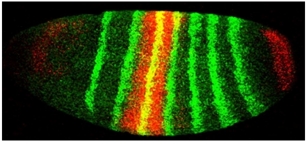


Figure: *Drosophila M.* segments

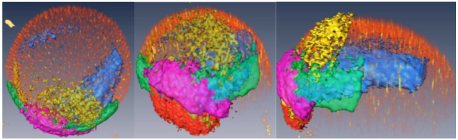


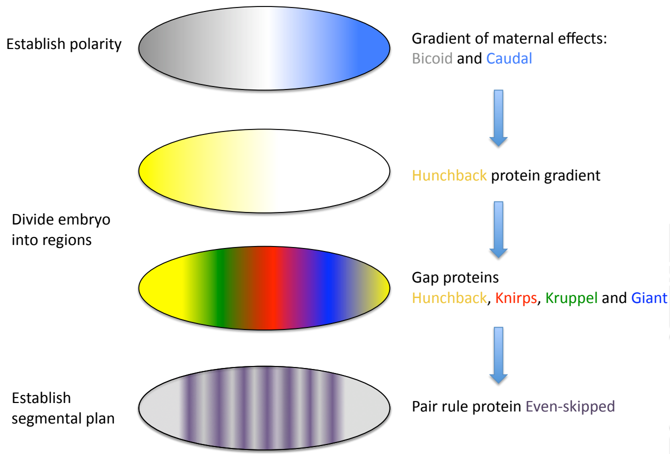
Figure: *Zebrafish* regionalisation [Castro Gonzalez et al., 2009]

- developmental biology recognise as important actors in the emergence of embryonic patterning—self-organised structures
  - transcriptional control mechanisms
  - signalling pathways
  - cell-to-cell direct interaction
  - short and long range signals (*morphogenes*)

$\rightarrow$ interplay between cells internal activity and cell-to-cell interactions

Biological Background - Gene Expression Pattern

- egg of Drosophila already polarised by maternal effects



Goal of the Model

- reproducing the expression pattern of the gap genes at Cl. Cyc. 14
- beginning with expression data at Cl. Cyc. 11
- experimental data and acquired images comes from the open on-line database FlyEx [2]

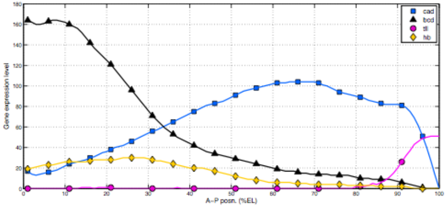


Figure: Quantitative experimental data at cl.cyc.11

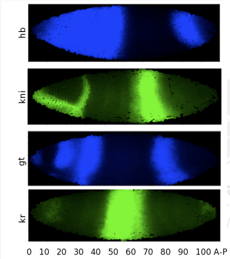


Figure: 2D image at cl.cyc.14

[2] http://flyex.ams.sunysb.edu/flyex/index.jsp

Model of the Cellular-System [Montagna et al., 2010]

- each cell is modelled as an agent
  - agent internal behaviour models GRN
  - agent interactive capabilities model cell-to-cell / cell-environment communication
  - agent replicates so to model cell mitosis
- the extra-cellular environment is modelled as a grid-like environment
  - grid grows with the number of cells
  - Hb, Kr, Kni and Gt are able to diffuse
  - concept of gradient

Qualitative Simulation Results at the Cl. Cyc 14 tc 8

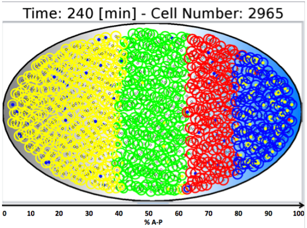


Figure: Gap gene expressions: *hb* (yellow), *kni* (red), *gt* (blue), *Kr* (green)

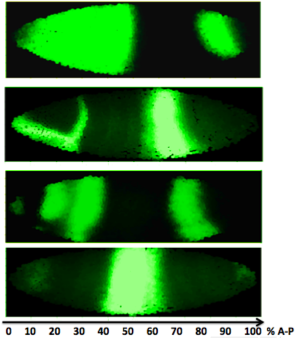
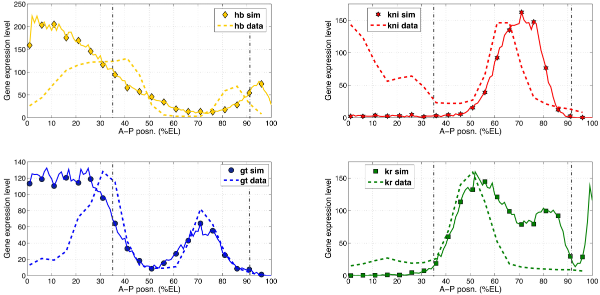


Figure: The experimental data for the expression of (from the top) *hb*, *kni*, *gt*, *Kr* ©Maria Samsonova and John Reinitz

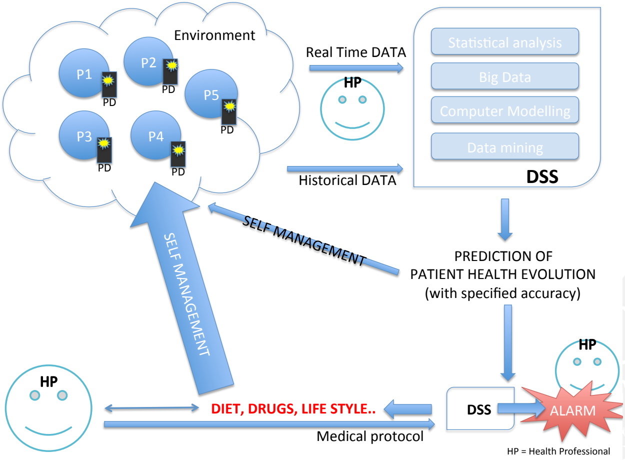
Quantitative Simulation Results [Montagna et al., 2015b]

Results at the Cl. Cyc 14 tc 8



Focus on. . .

Self-management of Health Conditions

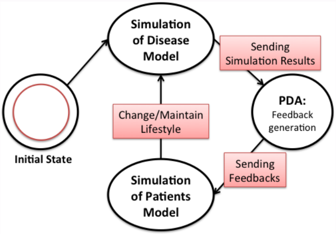


An Example on Type 1 DM Self-management

Goal

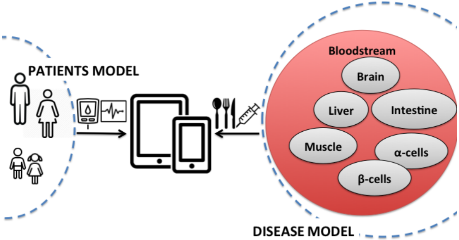
- to find solutions for identifying personalised therapies and lifestyle suggestions for patients to improve their outcome

Proposal



- we present an ABM of chronic disease self-management
  - from an initial state that reproduces the health condition of a patient
  - . . . a low level simulation of the metabolic system is performed
  - from the simulation results, feedbacks are provided to the patient

Two-Levels Model



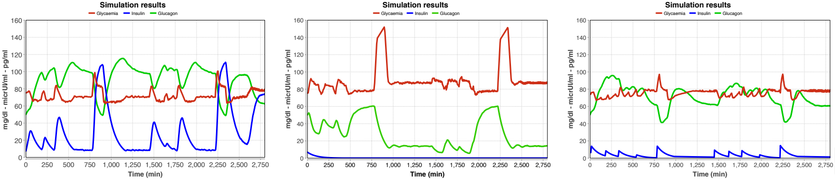
High-level: self-management model

- Patients are agents that behaves according to feedbacks received by their PDAs

Low-level: disease model

- Metabolic system as a set of interacting agents
  - each agent is a set of cells conducting the same activities
  - agents interact via an interaction medium, the environment, that models the bloodstream where agents release and retrieve molecules

Simulation Results

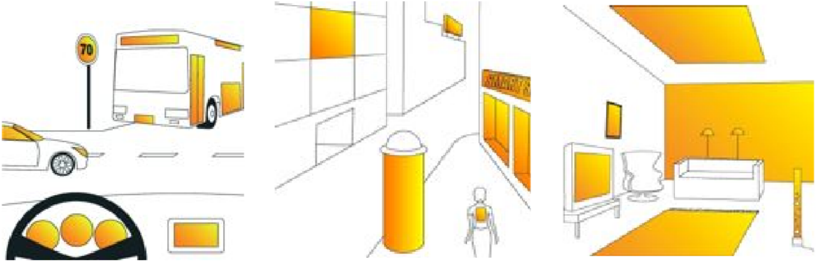


(a) Healthy patient (b) Type 1 DM patient (c) Self-managed patient

Figure: Glycaemia, insulin, and glucagon dynamic over two days of simulation in different conditions

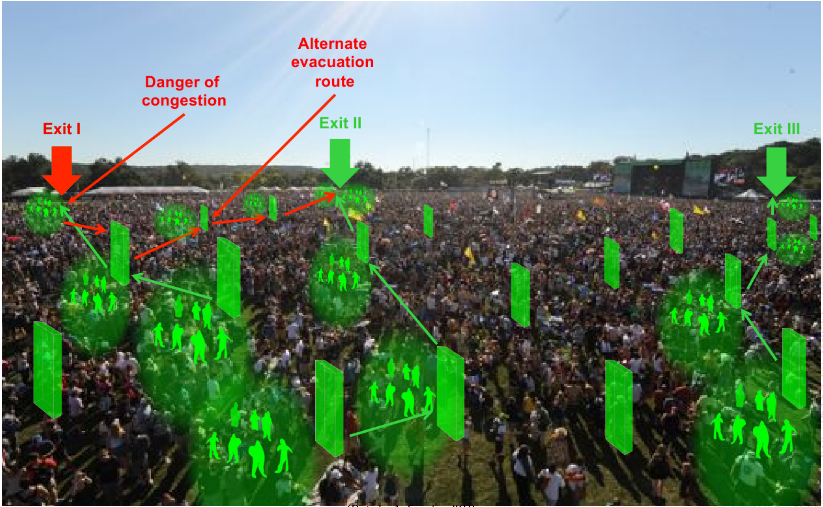
Focus on. . .

Our Starting Point: Tomorrow Pervasive Environments



(Pict. by A. Ferscha, JKU)

The Case of Crowd Engineering: The SAPERE project

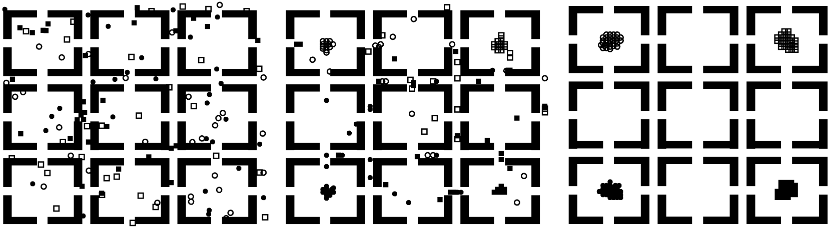


(Pict. by A. Ferscha, JKU)

A Crowd Steering Scenario: Guide Me to my Goal

Scenario description [Pianini et al., 2011]

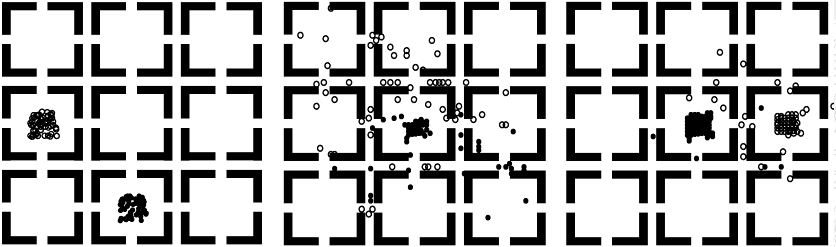
- system of nine halls, some of them contain points of interest
- people spread in the environment with smartphones
- each one has a goal, but doesn't know where to go
- everybody must be guided to the goal, avoiding crowded paths



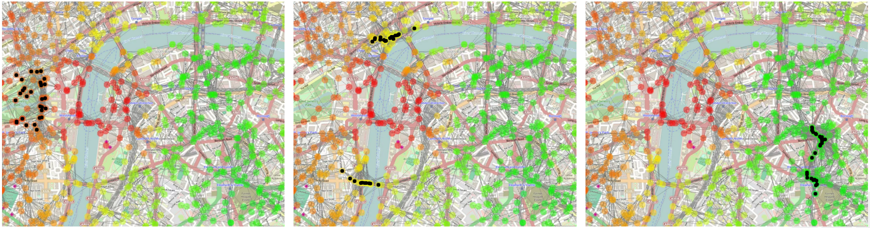
Let's Go See That! Avoid Overcrowded Areas

Scenario description [Pianini et al., 2011]

- same environment, with two groups of people
- black guys want to see something which is right in the middle of the ideal path for the whites towards their goal
- because of crowding avoidance, white guys reach their destination using secondary paths



Crowd-sensitive User Steering in London [Montagna et al., 2015a]



(a) Initial (b) Ongoing (c) Near-end

Figure: Three snapshots of the simulation. Our altered distance metric (the gradient) goes from green (most favourable and close to destination) to red (unpleasant or far from destination). Agents (in black) climb this structure towards greener values.

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