

Simulation & Multi-Agent Systems

An Introduction

Multiagent Systems LM

Sistemi Multiagente LM

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Ingegneria Due

ALMA MATER STUDIORUM—Università di Bologna a Cesena

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- 1 Simulation
 - Meaning, Motivation & Application
- 2 Types of Simulation
 - Micro, Macro and Multi-level Simulation
- 3 A Methodology
 - Domain, Design, Computational Model
- 4 Traditional Model and Simulation
 - Differential Equations: ODE, PDE, Master Equations
 - Computational Models
- 5 Agent-based Model and Multi-agent based Simulation
 - Why do we Need ABM?
 - What are ABM and MABS?
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 - How to implement ABM?
 - Applications of ABM
- 6 A Case Study
 - The Morphogenesis of Biological Systems
 - A Crowd steering scenario



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Scientific Method

Traditional science workflow [Parisi, 2001]

- Traditional scientific method
 - 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 / invalidation of theories



What Does it Happen 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 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
 - impossible to predict a-priori the evolution of the system



What Can we Do for. . .

- Making prediction 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 real system
 - analysing the effects of manipulating experimental conditions without having to perform complex experiments



Definition of Simulation

- Simulation is introduced as a new way for describing scientific theories

[Parisi, 2001]

- Simulation is the process with which we can study the dynamic evolution of a model system, usually through computational tools

[Banks, 1999]

- Simulation is the imitation of the operation of a real-world process or system over time



Simulation Requires a Model

M. Minsky – Models, Minds, Machines

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 .

- A model is a representation / abstraction of an actual system
- A model is a formalisation of aspects of a real process that aims to precisely and usefully describe that real process
- A model involves **aggregation**, **simplification** and **omission**
- The model implements theories which have to be verified during the simulation

Typical questions in model construction

- How complex should be the model?
- Which assumptions should be done?

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From Model to Simulation. . .

Computer simulation

- Models are designed to be run as processes within a computer
- Simulation creates a **virtual laboratory**
 - virtual phenomena observed under controlled conditions
 - possibility to easily modify the components of an experiment (variables, parameters, simulations' part)
- Subsequent simulations imitate the operations of the modelled process
 - generation of an artificial evolution of the system

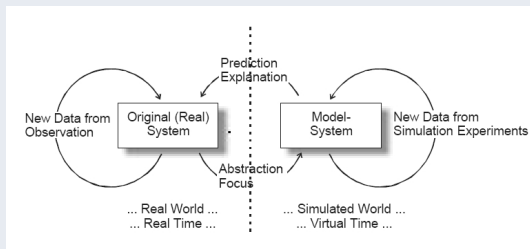


... and Back

- The observation of the evolution carries out deductions on the actual dynamics of the real system represented
- Simulation results make it possible to evaluate theories constructing the model

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



Applications of Simulation

- Interdisciplinary domain
- Complex Dynamical Systems
 - Biological systems (brain, biomolecular/cellular biology)
 - Clinical healthcare
 - Social systems
 - Ecosystems
 - Economic systems
 - Coordinating systems (swarm, flocking)
 - ...

→ systems too complex to be understood from observations and experiments alone

→ systems that does not exist and, for instance, has to be built

A multi-disciplinary research field

Maths, Physics, Informatics, Biology, Economy, Philosophy, ...

Features of Complex Systems in a Nutshell

Emergent phenomena which result from the interactions of individual autonomous entities → the whole is more than the sum of its parts

- Nonlinear dynamics
- Presence of positive and negative feed-backs
- Ability of evolution and adaptation
- Robustness
- Self-organisation
- Hierarchical organisation
- Eventually adaptation



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Granularity of Simulation Elements: 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 this entity
- Modelling, simulating and observation happens on one level: the *global level*
- The characteristic of a population are averaged together



Granularity of Simulation Elements: 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 thought as comprising 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 for reflecting emergent phenomena



Granularity of Simulation Elements: 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
- The system is described at different time scales

Advantages of Multi-level simulation

- It facilitates taking spatial and temporal structured processes into consideration
- It model the complex systems hierarchical organisation
- It allows the description of upward and downward causation



Down-ward and Up-Word Causation

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).^a

^aF. Heylighen. <http://pespmc1.vub.ac.be/DOWNCAUS.html>



How To Choose Between Different Approaches

Which kind of simulation?

- Modelling and simulating approaches are chosen on demand and thus address the diverse needs of modelling and simulation of the systems
- Multi-level simulation is considered the most suitable approach for studying complex systems



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Simulation Workflow

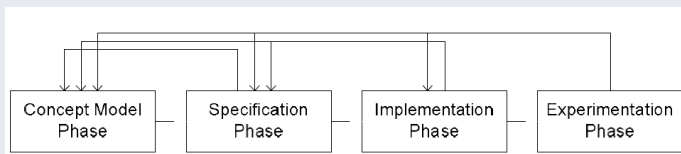
Main steps in a simulation study [Klugl and Norling, 2006]

- 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 a simulation of the model that can be executed on a computer
- Analysing simulation outputs
 - model validation and verification



How to Build a Model: Methodology

Model design



- Concept model phase – *Domain model*
 - Analysis of the real system characteristic
- Specification phase – *Design model*
 - translation of the information from the needs' into a formal model
 - aim: build a model independent of any tool and any software platform
- Implementation phase – *Computational model*
 - translation of the model resulting from the design on a particular software platform

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Differential Equations

- System described by a set of state variables
- Different types of differential equations
 - ODE — how do they vary in time
 - PDE — how do they vary in time and space
 - SDE — which is the probability that the variable has a certain value
- Time-dependent variables are assigned to different measuring 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.

Features

- Continuous Model
- Deterministic or Stochastic Model
- Macro Model

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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 $\{X_1, X_2, \dots, X_n\}$ 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 form, through a mathematical expression (ODE):

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

- 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
 - $\gamma_1, \gamma_2, \dots, \gamma_m$, are the parameters of the problem (*control parameters*)

Simulation of Differential Equations Models (I)

Analytical solution of differential equations

- Exact solution of a class of differential equations
- It is possible under very special circumstances
 - i.e. when the function F_j 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 $\{X_1, X_2, \dots, X_n\}$ for \mathbf{X}
- Time step is reduced to arbitrary small discrete intervals: values at consecutive time-points t_0, t_1, \dots, 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 $t \rightarrow \infty$
 - 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

Please remind

- 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
 - down-ward and up-ward systems dynamics
- Remind them if you wish to model a complex system
- They are important 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 established framework
 - They are relatively simple
 - They have a strong formal aspect
-
- Where do differential equations fail?



Analysis of Differential Equations II

Are they able to capture complex systems features?

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



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Computational Models

- Graphs and Networks
 - boolean networks
- Petri-Nets
- Stochastic- π -calculus
- Cellular Automata
- Agent-based Model



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Why do we Need Agent-Based Model (ABM)?

To... [Sun and Cheng, 2000, Bonabeau, 2002, Macal and North, 2006, Macal and North, 2010]

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



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What is Agent-based Model

Agent-based model 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.

- MAS provides designers and developers with. . .

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

Society — . . . a way of representing a group of entities whose behaviour emerges from the interaction among elements

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

Execute an ABM

- Running an ABM
 - computational engine for simulating agent behaviours and interactions
- Study 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



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When to Use Agent-based Model

- 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
- When the system consists in mutable interacting participants
 - agents can be erased
 - new agents can enter in the scenario
- When averages will not work



Advantages and Problems of Agent-based Model

• Advantages

- 1 It captures emergent phenomena
- 2 It provides a natural description of a system
→ it makes the model seem closer to reality
- 3 It is flexible

• Problems

- 1 There is a lack of
 - an unified formal framework for unambiguously representing ABM elements and rules
 - a widely accepted methodology for developing MABS
- 2 It increases the amounts of parameters
- 3 Software development remains a significant barrier to the use of ABM
 - inconsistency and incongruence between agents of the conceptual model and agents of the computational model



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Defining Agents of an ABM

Identifying agents, accurately specifying their behaviours, and appropriately representing agent interactions are the keys for developing useful ABM

An Agent in ABM requires mechanisms for

- Receiving the input e.g., through **sensors**
- Storing history, e.g., through a **state**
- Autonomously devising next action, e.g., through decision rules which define the
 - 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

→ processing the ability of adapting to changing environment



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Multi-Agent Based Simulation Platforms

Agent-based toolkits providing frameworks and libraries that simplify the procedures of establishing models and performing simulations

Standard issues [Railsback et al., 2006]

- Model structure, i.e. agent behaviour, agent communication mechanisms, environment and topology
- Discrete event simulation
 - *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



Swarm

Swarm <http://www.swarm.org/>

- Objectives
 - to ensure a widespread use across scientific domains
 - to implement a model
 - to provide a virtual laboratory for observing and conducting experiments
- Swarm is implemented in Objective-C

Java Swarm

- Set of Java classes that allow the use of Swarm's Objective-C libraries from Java



Repast

Repast <http://repast.sourceforge.net/>

- Objectives
 - to implement Swarm in Java
 - to support the specific domain of social science (it includes specific tools to that domain)
 - to make it easier for inexperienced users to build models

Repast is free and open source



MASON

MASON <http://cs.gmu.edu/~eclab/projects/mason/>

- Objectives
 - models with many agents executed over many iterations
 - to maximize execution speed
 - to assure complete reproducibility across hardware
 - to detach or attach graphical interfaces
 - to be not domain specific
- Basic capabilities for graphing and random number distributions



Limitations of these Platforms

- Difficulty of use
- Insufficient tools for building models
- Lack of tools for documenting and communicating software
- Incoherence between the design model and the computational model
 - computational agents \neq conceptual agents
 - no first-class abstraction for modelling the environment



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



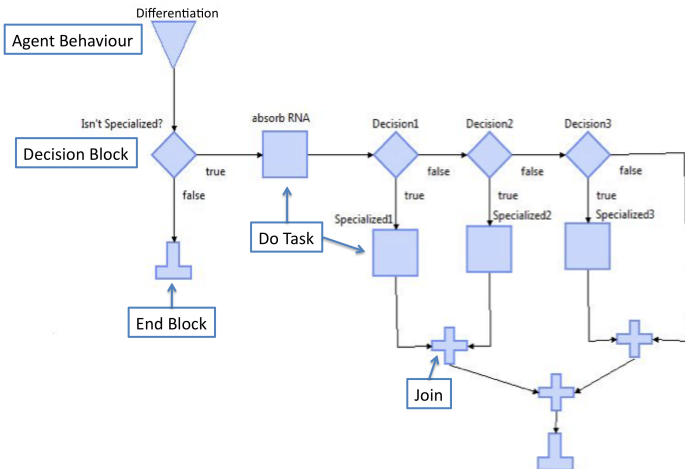
More Details on Repast Symphony

- 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 including R, VisAD, Weka, popular spreadsheets, MATLAB, and iReport
- A flexible definition of space for modelling and visualise 2D and 3D environments
- A fully concurrent multithreaded discrete event scheduler
- Libraries for genetic algorithms, neural networks, regression, random number generation, and specialized mathematics
- Automated Monte Carlo simulation framework



Creating a Repast Model with the Visual Agent Editor

- for more details see the on-line tutorial
<http://repast.sourceforge.net/download.html>



Creating a Repast Model with Java Objects

- 1 **ContextBuilder** defines the main components of the system
 - the environment (with the number and dimension of the grids) where the agents can move
 - the type and initial number of agents that populate the environment
- 2 **Agent Classes** such **SimpleAgent**
 - the core method is `step` which precedes methods to be scheduled
 - it has several options: start time, the updated interval
 - it is override by the subclasses



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Applications of ABM

- 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 ...



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On the Morphogenesis of Living Systems

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



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

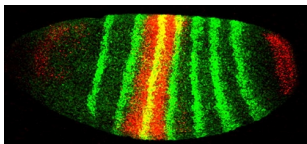


Figure: *Drosophila M.* segments

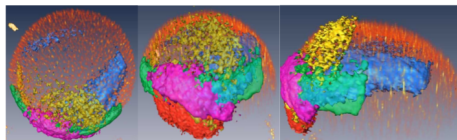


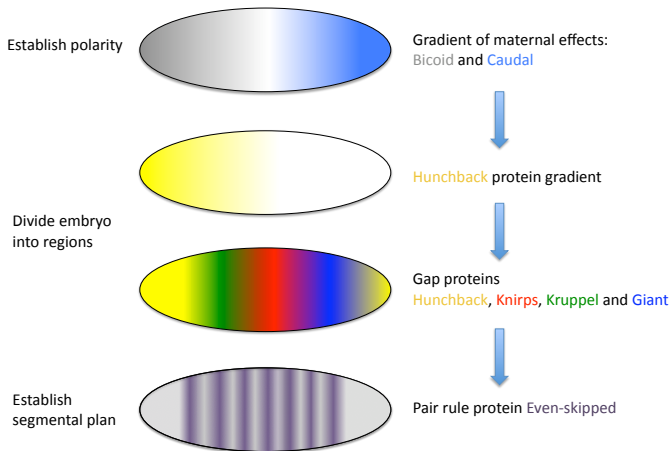
Figure: *Zebrafish* regionalisation
[Castro Gonzalez et al., 2009]

- 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*)
- 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 FlyEx¹

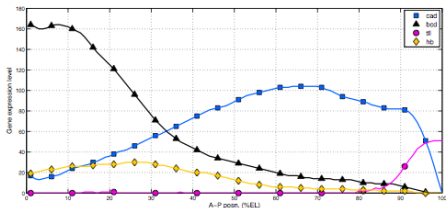


Figure: Quantitative experimental data at cl.cyc.11

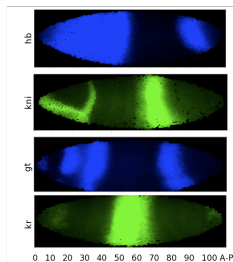


Figure: 2D image at cl.cyc.14

¹ <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



Model Implementation and Simulation Procedure

- The model is implemented on top of Repast Simphony²
 - open-source agent-based modelling and simulation toolkit
 - abstraction for modelling the agent behaviour and the environment
 - multithreaded discrete event scheduler
- Simulations
 - are executed from the cleavage cycle 11
 - a time step corresponds to 4 seconds of the real system simulated

²<http://repast.sourceforge.net/index.html>



Qualitative Results

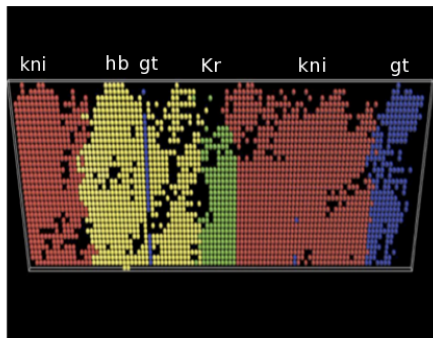
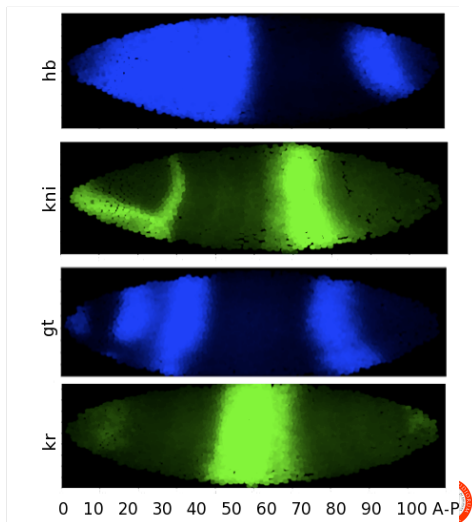


Figure: Qualitative results charted in 2D at the eighth time step of cleavage cycle 14A. The image shows for each cell of the embryo the genes with higher expression.



Outline

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- 2 Types of Simulation
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- 4 Traditional Model and Simulation
 - Differential Equations: ODE, PDE, Master Equations
 - Computational Models
- 5 Agent-based Model and Multi-agent based Simulation
 - Why do we Need ABM?
 - What are ABM and MABS?
 - When to use ABM?
 - How to use ABM and MABS?
 - How to implement ABM?
 - Applications of ABM
- 6 A Case Study
 - The Morphogenesis of Biological Systems
 - A Crowd steering scenario

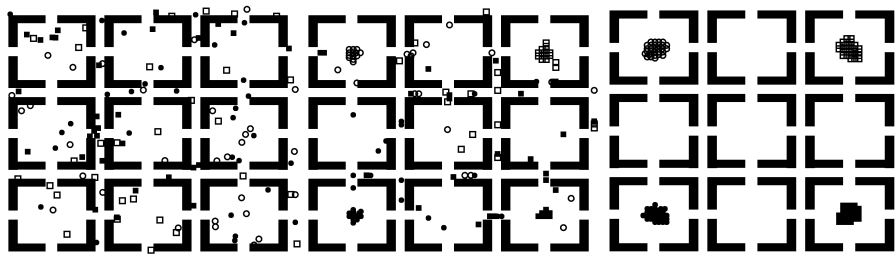


A Crowd Steering Scenario: Guide me to my Goal

[Pianini et al., 2011]

Scenario description

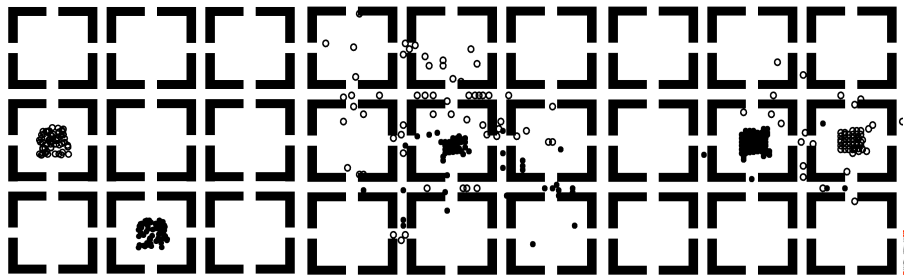
- System of nine halls, some of them contain points of interest
- People spread in the environment with smartphones
- Each one has a goal, but doesn't know where to go
- Everybody must be guided to the goal, avoiding crowded paths



Let's go see that! Avoid overcrowded areas

Scenario description

- 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



Available Projects and Thesis

- Modelling bio-staff
 - going ahead with developmental biology scenarios
 - modelling signalling pathways (in collaboration with Prof. Pedro Pablo González Pérez – Universidad Autónoma Metropolitana, Ciudad de México)



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An Introduction

Multiagent Systems LM

Sistemi Multiagente LM

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