Simulation & Multi-Agent Systems
An Introduction

Multiagent Systems LM
Sistemi Multiagente LM

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Academic Year 2010/2011

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

Definition of Simulation

- 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

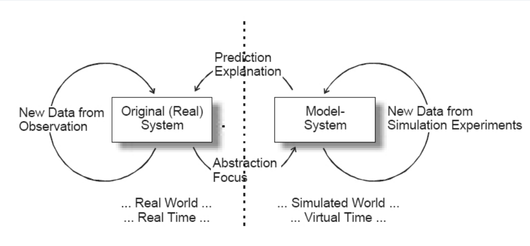
- Models are designed to be run as processes within a computer
- Simulation creates a virtual laboratory
  - virtual phenomena observed under controlled conditions
  - possibility to easily modify the components of an experiment (variables, parameters, simulations' part)
- Subsequent simulations imitate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



Why do we Need Simulations?

[Parisi, 2001, Klugl and Norling, 2006]

- The simulated 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 Simulations are Used 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

Applications of Simulation

- Interdisciplinary domain
- Complex Dynamical Systems
    - Brain
    - Social Systems
    - Ecosystems
    - Economic Systems
    - Coordinating Systems (swarm, flocking)
    - ...

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

A multi-disciplinary research field

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

Features of Complex Systems in a Nutshell

- Nonlinear dynamics
- Presence of positive and negative feed-backs
- Ability of evolution and adaptation
- Robustness
- Self-organisation
- Hierarchical organisation
- Emergent phenomena which result from the interactions of individual entities → the whole is more then the sum of its parts

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]

[a] F. 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

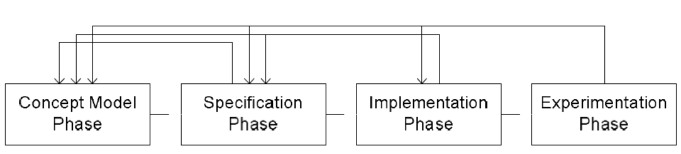
Simulation Workflow

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

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

- Continuos 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 $\{X_1, X_2, ..., X_n\}$ 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):

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

- 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

- Exact solution of a class of differential equations
- It is 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

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

Computational Models

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

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

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

1. . . . model the individual properties thet 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

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
- 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

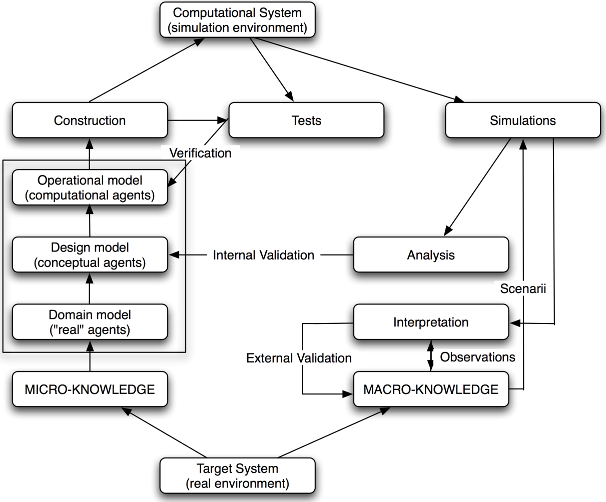
When to Use Agent-based Model

- 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
     $\rightarrow$ 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
     - inconsistence and incongruence between agents of the conceptual model and agents of the computational model

The Methodology in a Figure



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
- Devising next action, *e.g.*, through decision rules which define the
  - reactive behaviour — how an agent reacts to external stimuli
  - 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

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*: controling which specific actions are executed and when (in simulated time)
  - *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

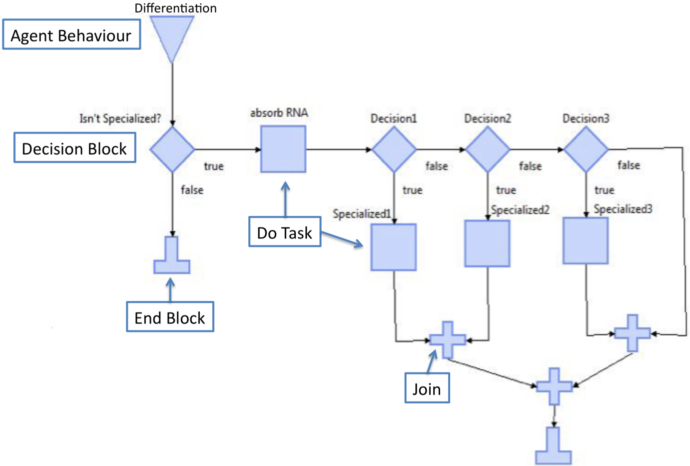
Coherence between design and computational model still missing

More Details on Repast Simphony

- 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

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

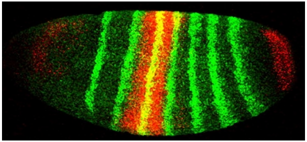


Figure: *Drosophila M.* segments

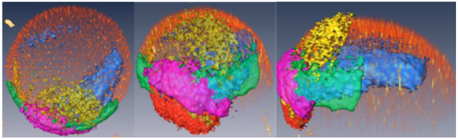


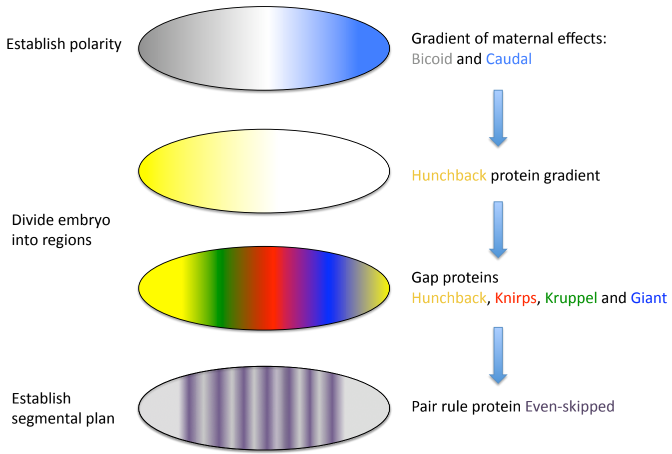
Figure: *Zebrafish* regionalisation [Castro Gonzalez et al., 2009]

- 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 gene expression pattern of the gap genes at Cleavage Cycle 14A - temporal class 8...
  - *hunchback* (hb), *Krüppel* (Kr), *knirps* (kni) and *giant* (gt)

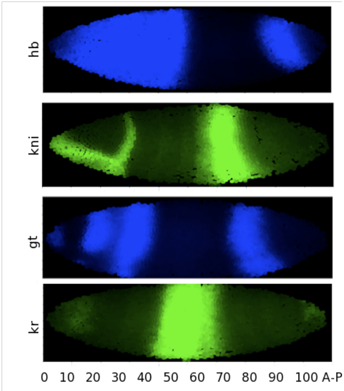


Figure: 2D data from the FlyEx database[1]

Initial Condition

- ... Beginning with expression data at Cleavage Cycle 11

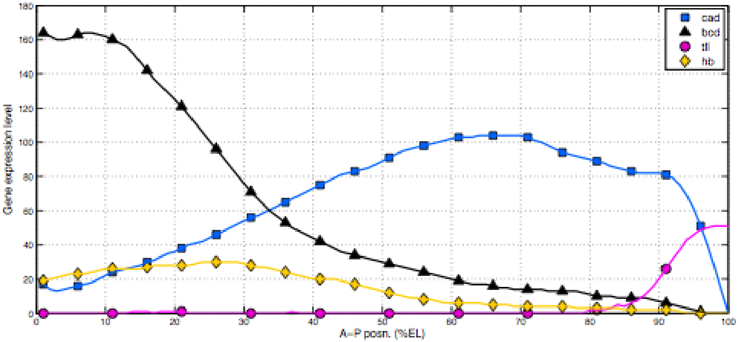
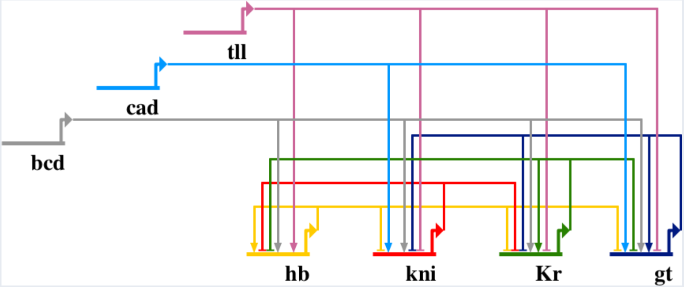


Figure: Experimental data from the FlyEx database of genes with non-zero concentration. The concentration of proteins are unitless, ranging from 0 to 255, at space point x, ranging from 0 to 100 % of embryo length.

The Intracellular Network Structure

- *caudal* and *bicoid* are maternal effectors
- They drive the expression of the gap genes *hunchback* (hb), *Krüppel* (Kr), *knirps* (kni) and *giant* (gt)
- *tailess* (tll) is a gap gene that we model as an input of the network

Intracellular network from literature [Perkins et al., 2006]



Model of the Cellular-System

- 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 of the Cell

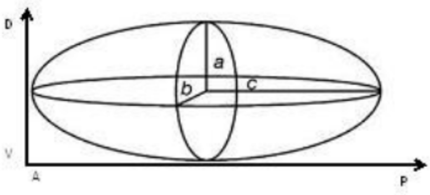
- Gene regulatory network – agent behaviour
  - gene transcription might be activated or repressed
  - activation/inhibition is stochastic and depends on the concentration of transcription factors

$$P_{hb} = f([Bicoid]) + f([Hunkbuck]) + f([Tailess]) - f([Knirps]) - f([Kruppel])$$

  - f is a linear function with the proportionality constant representing the strength of interaction
  - if $P_{hb} > 0$ the protein is synthesised, otherwise the gene remains silent
- Mitosis
  - agents replicate according to the rate of cell division
- Chemical diffusion – agent interaction with the environment
  - chemicals are absorbed or released from/to the same location of the grid-like environment

Model of the Environment

- 3D tapered structure of the embryo → 2D section along the antero-posterior axis (c)
- Space is not continuous but grid-like
  - in each location a cell and/or morphogens
- Environment dynamic
  - diffusion of morphogens from region with bigger concentration to region with lower concentration, according to the *Fick's low*



Model Implementation and Simulation Procedure

- The model is implemented on top of Repast Simphony[2]
  - 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

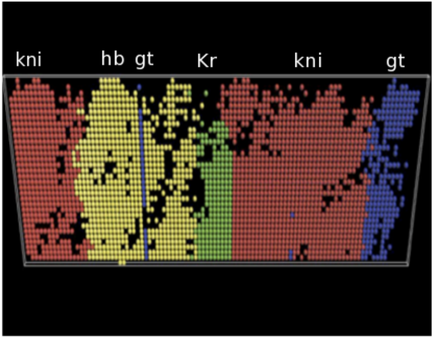
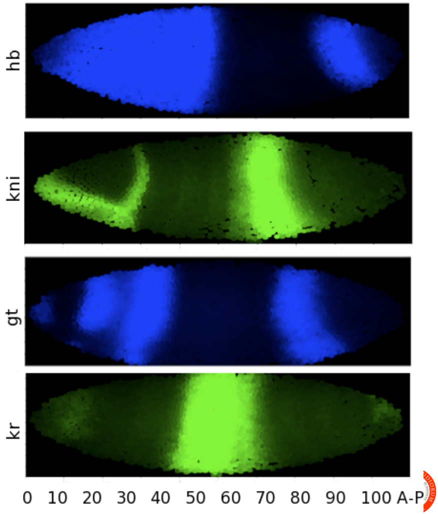


Figure: Qualitative results charted in 2D at the eighth time step of cleavage cycle 14A. The image shows for each cell of the embryo the genes with higher expression.



Quantitative Results

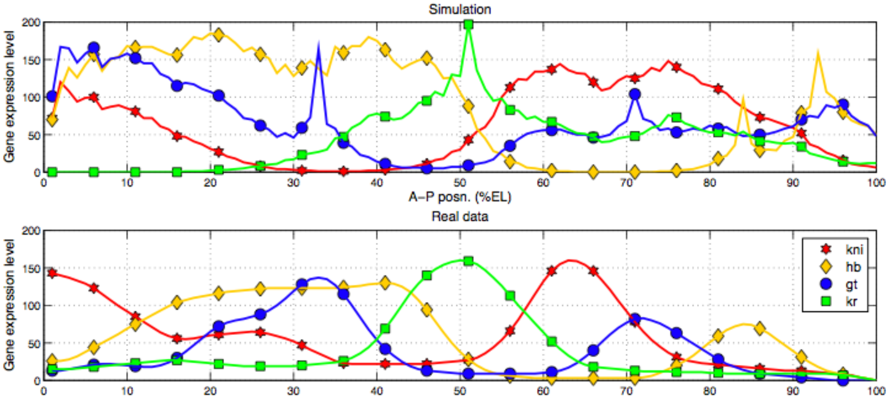


Figure: Quantitative simulation results for the four gap genes *hb, kni, gt, Kr* at a simulation time equivalent to the eighth time step of cleavage cycle 14A (top) and the corresponding experimental data (bottom)

Bibliography I

Banks, J. (1999).
Introduction to simulation.
In Farrington, P., Nembhard, H. B., Sturrock, D. T., and Evans, G. W., editors, *Proceedings of the 1999 Winter Simulation Conference*, pages 7–13.

Bonabeau, E. (2002).
Agent-based modeling: Methods and techniques for simulating human systems.
PNAS, 99(suppl. 3):7280–7287.

Bibliography II

Castro Gonzalez, C., Luengo-Oroz, M. A., Desnoulez, S., Duloquin, L., Fernández-de Manuel, L., Montagna, S., Ledesma-Carbayo, M. J., Bourgine, P., Peyrieras, N., and Santos, A. (2009).
An automatic quantification and registration strategy to create a gene expression atlas of zebrafish embryogenesis.
In *31st Annual International Conference of the IEEE EMBS*, pages 1469–1472, Minneapolis, Minnesota, USA.

Klugl, F. and Norling, E. (2006).
Agent-based simulation: Social science simulation and beyond.
Technical report, The Eighth European Agent Systems Summer School (EASSS 2006), Annecy.

Bibliography III

Macal, C. M. and North, M. J. (2006).
Tutorial on agent-based modeling and simulation part 2: how to model with agents.
In *WSC '06: Proceedings of the 38th conference on Winter simulation*, pages 73–83. Winter Simulation Conference.

Parisi, D. (2001).
Simulazioni - La realtà rifatta al computer.
Società editrice il Mulino.

Perkins, T. J., Jaeger, J., Reinitz, J., and Glass, L. (2006).
Reverse engineering the gap gene network of *Drosophila Melanogaster*.

PLoS Computational Biology, 2(5):e51.

Bibliography IV

Railsback, S. F., Lytinen, S. L., and Jackson, S. K. (2006).
Agent-based simulation platforms: Review and development recommendations.
Simulation, 82(9):609–623.

Sun, Y. and Cheng, L. (2000).
A survey on agent-based modelling and equation-based modelling.
In *Proceedings of Department of Computer Science (Georgia State University)*.

Uhrmacher, A. M., Degenring, D., and Zeigler, B. (2005).
Discrete Event Multi-level Models for Systems Biology.
In Priami, C., editor, *Principles of Organization in Organisms: Proceedings of the Workshop on Principles of Organization in Organisms*, volume 3380 of *Lecture Notes in Computer Science*, pages 66–89. Springer.

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