

COMP6216

# Simulation Modelling for Computer Science

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# Me

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- Part of the “Complexity” part of the AIC (Agents, Interaction, Complexity) group
- Research interests in
  - (evolutionary) game theory
  - Networks (structure + function)
    - For analyzing data and building models to understand data (twitter networks + ED, language)
    - As abstract models (spatial networks)
    - Models of the banking system, cascading
  - Dynamical Systems on Networks (mostly related to synchronization and evolutionary games)

# If you are interested in doing a PhD

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- I have a project on modelling cascading failure in the banking system
  - Networks of interconnected banks
  - Adjustable risk taking (game theory)
  - Optimal intervention strategies?
  - Via NGCM CDT <http://www.ngcm.soton.ac.uk/>
  - More info: <https://jobs.soton.ac.uk/Vacancy.aspx?id=12152&forced=1>
- Also interested in potential PhD students who want to work on data mining and network analysis related to health (using twitter information)

# You?

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- I don't really know
  - CS Msc? 3<sup>rd</sup> year BSC?
  - Spitfire?
  - Other?
- Also:
  - This is a fairly new module and I am not so sure what you already know. Tell me when I am too fast or too slow ...

# Requirements

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- A bit of maths: mostly differential + integral calculus, Taylor expansions, ...
- Some programming experience
- Will try to find a balance between teaching
  - mathematical treatment
  - numerical implementation
  - general modelling skills... and have interesting applications.  
(Let me know if there is anything you are particularly interested in, I can try to include it)

# The Module – COMP6216

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- Logistics:
  - 2 lectures per week/1 seminar per week
  - Rooms:
    - Tuesdays 9-10 27/2001/LR1 (Lecture)
    - Tuesdays 3-4pm 58/1009 (Seminar – not 1<sup>st</sup> week!)
    - Thursdays 3pm-4pm 07/3031 (Lecture)
  - Website:<http://users.ecs.soton.ac.uk/mb8/sim/sim.html>
- Simulation Modelling, three aspects will be covered
  - Modelling
  - Scientific Computing
  - Applications of Simulation Modelling

# Modelling

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- The aim is to understand the role of modelling in science and to learn how to build a (good) model
- Aspects covered:
  - What is science? What is the role of models in science?
  - How to build a model
  - Practical aspects of modelling
  - An introduction to a selection of modelling paradigms

# Scientific Computing

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- The aim is to understand some important numerical techniques to “solve” models using computers
  - Solving (non-)linear equations
  - Calculating derivatives/integrals
  - Solving ordinary differential equations
  - Agent-based models
  - Networks
  - Potentially: Optimization, Monte Carlo Methods



# Applications

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- Will have a look at a number of applications from various fields to introduce and apply concepts
  - Some physics ... how cats fall, the dynamics of love affairs, and more boring stuff
  - Population models in biology ... a lot about populations of bacteria
  - Epidemiology ... how diseases spread and zombie apocalypses can be prevented
  - The WWW ... can we understand and model the large scale structure of the internet? Ranking web pages and scientific papers.
- Will also look at some specific modelling platforms

# Types of Models

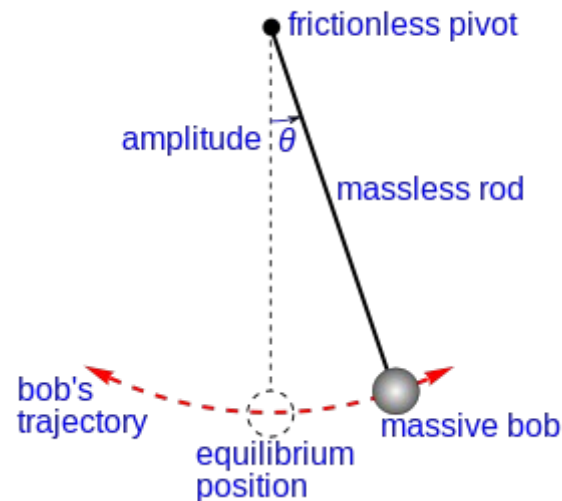
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- Statistical Models
  - Start with data, build regression models to fit data and correlation in data
  - Correlation-causation?
  - Only a bit of Monte Carlo covered in this module
- Instead, focus will be on “Dynamical Models”
  - Describe system state, rules for evolution, and investigate outcome of these rules
  - Dominant paradigm in natural science
  - Will focus on this in this module
  - “Evolution rules” often captured by differential equations -> need to learn something about them.

# Example

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- A pendulum



## Statistical Model

Start with series of observations of ,e.g., length of period and length of rod -> fit dependency and conclude  $T \sim \text{square root of } L$

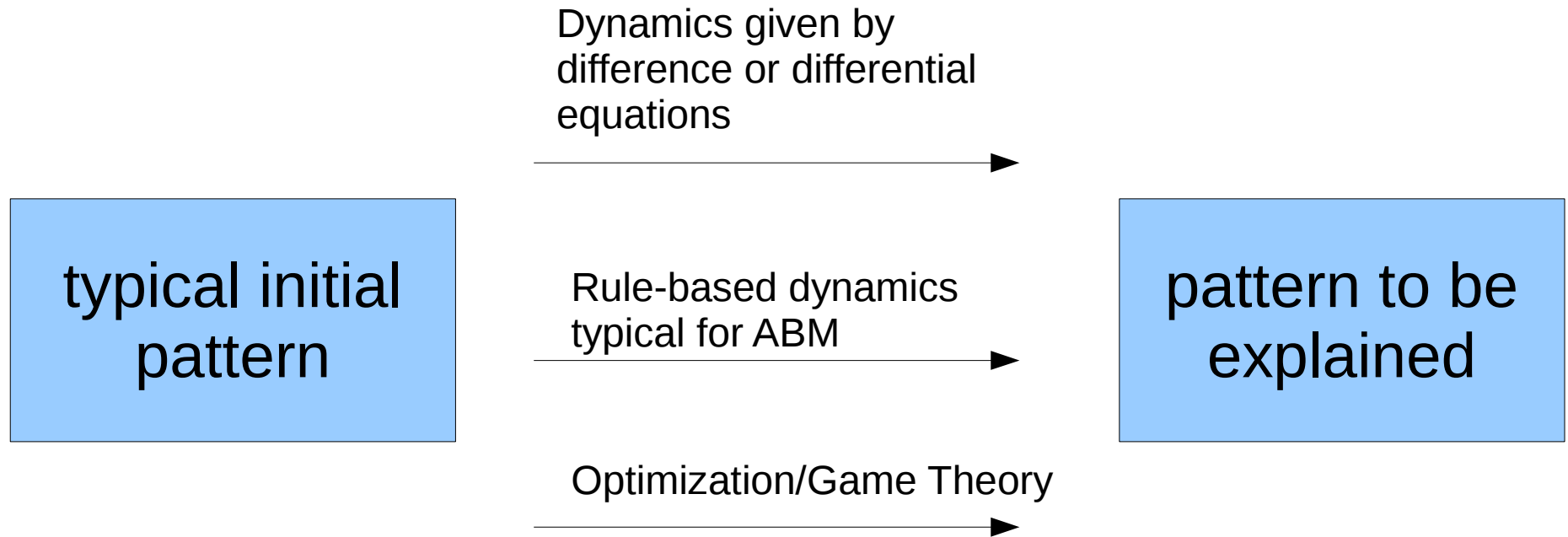
## “Dynamical Model”

Build model based on Newton's Laws, solve differential equation, conclude  $T \sim \text{square root of } L$  as a property of solutions

# Typical Situation

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- Observe some pattern (in the real world), want to explain how it arose.



# Difference/Differential Eq's

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- Time in evolution rule can be
  - discrete (-> difference equations, clocked time)

$$x_{t+1} = f(x_t, t)$$

- or continuous (-> differential equations)

$$dx/dt = f(x, t)$$

- Thinking about populations, a system can be composed of
  - Many similar entities (somehow well mixed) -> differential equations
  - Heterogeneous entities, possibly not very many -> agent-based models

# Examples

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- Computer operations -> clocked time, difference equations
- The pendulum -> continuous time -> differential equations
- Population dynamics of a huge herd of cattle -> differential equations
- Dynamics of this class -> Agent-based model
- Disease spread in large populations of humans
  - Depends.
    - Traditionally: differential equations.
    - But some details do matter -> ABM

# Plan of the Course

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- First part: Lectures on Scientific Computing
  - basic numerical methods,
    - Next week: equation solving (linear + non-linear),
    - Then: Taylor expansions, numerical integration + differentiation, difference equations, ... etc.
- Second part:
  - Introduction to differential equations, some solution and analysis techniques + numerical methods to solve them
  - Intro to Mathematica/Matlab and system dynamics
  - Will connect this to applications

# Plan of the Course (cont.)

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- Third part:
  - Some modelling “theory” (+maybe role of modelling in science)
  - Agent-based models
  - Introduction to Netlogo and examples
- After that (time permitting):
  - Networks
  - Monte Carlo
  - Optimization



# Assessment

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- Two components
  - 30% Select a simulation modelling paper and give a 10 minute talk about it in the second half of the term (will be scheduled after Easter)
    - Describe the aim/purpose of the paper
    - Talk about the background and what the paper contributes to the field
    - Describe methodology and results
  - What matters to get a good mark:
    - Overall quality of the talk (did you speak well, quality of the slides, did you really understand the paper? Address all aspects mentioned above? Answer questions? ...)

# Assessment

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- Second component (70%) is implementing a model for one of the given problems, using various techniques to solve the model, and writing a 6 page conference paper documenting your results
- Marks are given for:
  - 10% quality of the report (writing, figures)
  - 40% technical quality (modelling techniques implemented properly, are results discussed and understood properly, see later)
  - 20% an extension of the given problem: Consider the given problem and develop an additional scientific question that makes sense in the given context and explore it adapting your models

# Assessment

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- For the second part you can also work on another problem (maybe related to your work/interests), but you need to discuss this with me
- Assessments due:
  - Your talk should be ready in the first week after Easter (April 18), can be scheduled any time after
  - The report is due at the end of the teaching period, May 13, 4pm.

# Some Suggestions for Papers for Part I of the Assessment

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- M. Nowak & R. May, “Evolutionary games and spatial chaos” (1992), *Nature* 359, 826.
- R. Cont & J.-P. Bouchaud, “Herd behaviour and aggregate fluctuations in financial markets” (2000), *Macroeconomic Dynamics* 4, 170.
- P. M. Todd et al., “Aggregate age-at-marriage patterns from individual mate search-heuristics” (2005), *Demography* 42, 559.
- N. Kashtan & U. Alon, “Spontaneous evolution of modularity and network motifs” (2005), *PNAS* 102, 13773.
- P. M. Allen & J. M. McGlade, “Modelling complex human systems: A fisheries example” (1987), *European Journal of Operational Research* 30, 147.
- A. Tero et al., “Rules for biologically inspired adaptive network design” (2010), *Science* 327, 439.

- G. Ichinose et. al., “Adaptive long-range migration promotes cooperation under tempting conditions” (2013), *Scientific Reports* 3, 2509.
- F. Simini et al., “A universal model for mobility and migration patterns” (2012), *Nature* 484, 96.
- S. Motesharrei et al., "Human and nature dynamics (HANDY): modeling inequality and use of resources in the collapse or sustainability of societies” (2014), *Ecological Economics* 101, 90.
- H. Berestycki et al. “Travelling Wave Solutions in a Reaction-Diffusion Model for Criminal Activity” (2014), *Multiscale Modelling and Simulation* 11, 1097.
- M. Bedau & N. H. Packard, “Evolution of evolvability via adaptation of mutation rates” (2003), *BioSystems* 69, 143.
- I. D. Couzin et al., “Uninformed individuals promote consensus in animal groups” (2011), *Science* 334, 1578.
- B. J. Dermody et al., “The evolutionary pathway to obligate scavenging in gyps vultures” (2011), *PloS ONE* 6, e24635.

# Paper Suggestions

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- Or basically any (at least moderately complex) modelling paper you like.
  - If in doubt, ask me, and I'll let you know if I think it is suitable.

# Part II Assessment

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- I will give you a problem
- You are supposed to:
  - Develop a differential equation based model – 7.5%
  - Explore analytical techniques to solve it (and if possible do so, if not, explain the difficulties) – 7.5%
  - Numerically integrate the equations using your own implementation of a solution method and compare to the analytical results -- 10%
  - Implement an agent-based model that addresses the same problem and compare its results to the above two results – 15%

# Part II Assessment

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- What should be in the report?
  - An description of the problem
  - Documentation of the analytical approach (such that I can follow every step and understand its logic)
  - Documentation of the application of the numerical integration methods (source code of the “essential bit” of your solver, choices and parameters you made for the solver and a brief explanation why, documentation and discussion of the comparisons you carried out)
  - Details of the ABM – how you implemented it and discussion of results and comparisons
  - Extension: Convince me it is interesting! Then document and discuss in detail what you did and document results in such a way that I can reproduce them.



# Part II Assessment

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- Also: upload the code for any numerical stuff you have done.

# Part II Assessment: Group Dynamics of Hard Workers and Lazy Workers

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- Consider the following situation:
  - A population of students is working on group projects. Students can follow two strategies (S): work hard for the project or free-ride.
  - In every course, groups of size  $n$  are formed at random. Students use the strategy determined at the beginning of the course (see below).
  - Total group effort is determined by the composition of the group. In a group with  $h$  hard workers and  $l=n-h$  lazy workers total group effort is  $e=h*H+l*L$  ( $H$  and  $L$  being the effort put in by hard/lazy workers)
  - When group projects are marked, every student gets the same mark. The lecturer determines this mark as  $m=e/n$  (i.e. the larger this number the better the mark)
  - At the end of the semester students rethink their strategies. They do this, by selecting another student at random and comparing a measure based on marks and effort,  $m-a*S$  (where  $a$  is a parameter and  $S=H$  or  $S=L$  depending on strategy). If that student got a measure, they will follow his strategy in the next semester.
  - Students study forever (i.e. take an infinite number of courses)

# Problem (cont.)

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- Q's:
  - Assuming we start with equal numbers of hard working and lazy workers, what is the composition of the group
    - After 4 years (i.e. 8 courses) if  $H=1$  and  $L=0$  and  $a=0.5$ .
    - in the long run (after an “infinite” number of years)?
    - How quickly is this equilibrium state reached?
  - How do the following parameters influence results:
    - Initial composition of the group
    - Group size ( $n$ )
    - Cost of effort  $a$
    - Contribution of hard workers to group effort (i.e.  $H$  and  $L$ )

# Assessment

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- Will use some of the seminar spots after Easter to answer questions/help with this part of the assessment of required