CITS4403
Computational Modelling

Lecture 1: Course Info & Complexity Science Overview

Dr. Siwen Luo

Semester 2, 2024
School of Computer Science,
University of Western Australia

LECTURE PLAN

Lecture 1: Course Info & Complexity Science Overview

1. **Course Introduction**
2. Computational Modelling
   - Simulation vs. Modelling
3. Complex System
   - Complex system features
4. Introduction of Complexity Science

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Dr Siwen Luo
Lecturer, University of Western Australia

Education

- PhD Computer Science (Artificial Intelligence), *The University of Sydney*

Teaching

- Computational Modelling – CITS4403
- Natural Language Processing – CITS4012
- Computer Analysis and Visualization – CITS2401

Research Experience

- Received **Top-tier AI Conferences Best Paper Award/Best Area Paper Award**
- Invited Reviewer of top-tier AI conferences
- Top-tier Information Retrieval Conference Workshop Chair

CITS4403 Computational Modelling

This unit is about complexity science, data structures and algorithms, intermediate programming in Python, and the philosophy of science.

We will explore research topics in computational modelling of complex systems, and you will develop skills to identify problems, formulate solutions and conduct further research in open questions in this domain.

Where to find the course information?

Unit Outline – CITS4403
https://lms.uwa.edu.au/bbcswebdav/institution/Unit_Outlines_2024/CITS4403_SEM-2_2024/CITS4403_SEM-2_2024_UnitOutline.html

LMS – CITS4403
https://lms.uwa.edu.au/ultra/courses/_91114_1/cl/outline

CITS4403 Computational Modelling

Learning Outcomes

On completion of this unit, students will be able to:

- *Present computational models to address a given research hypothesis and qualify the limitations of these models;*
- *Identify and discuss open research topics in the field of computational modelling;*
- *Explain the concepts and technologies used in the field of computational modelling;*
- *Design, apply and analyse relevant technologies to solve problems in the field of computational modelling.*

What will you learn in this course?

- Week 1: Introduction to Complexity Science
- Week 2: Graph I
- Week 3: Graph II
- Week 4: Cellular Automata I

- Week 5: Cellular Automata II
- Week 6: In-lecture Test
- Week 7: Agent-based Modelling I
- Week 8: Agent-based Modelling II

- Week 10: Evolution I
- Week 11: Evolution II
- Week 12: Self Organized Criticality & Exam Review

Assessment Overview

Assessment	Weight	Due
In-Lecture Test	25%	Week 6 (Monday, 26th August)
Group Project	25%	Week 12 (Monday, 14th October 11.59pm AWST)
Final Exam	50%	Exam Period

In-Lecture Test (25%)

This In-Lecture Test will be on-campus exam, held during the normal lecture time (***26th August 2024, 9am – 11am***). This test will examine over W1 to W5 contents.

You will be asked to answer variety of theoretical and coding questions.

Project Assignment (25%)

The focus of this assignment is to identify and discuss open research topics in the field of computational modelling, solve a computational modelling problem through designing and applying relevant algorithms and techniques, such as graphs, cellular automata and agent-based modelling etc. You are required to use Python to implement your algorithms and write the report to discuss your design, solution and findings.

***NOTE: This Assignment** would be a group assignment of **2 people**.*

Final Exam (50%)

The final exam will be an on-campus exam
You will be asked to answer variety of theoretical and coding questions.

Working Hours

- You are expected to work 12 hours per week for this unit.
- Attend 2 hours of lectures per week:
  - Monday 9AM – 11AM
  - Lectures are recorded, but please come to the lecture in-person as much as possible
- Attend 2 hour of laboratory; ***(NO lab in Week 1)***
- Read relevant chapters of textbook;
- Participate respectfully in discussions in lectures and labs;
- Complete all assessment tasks on time.

Full Course Timetable at course website:

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 AM			**CITS4403** (SEM-2) **Laboratory** MATH: [123B] **Wks** 30-35, 37-42		
9:00 AM	**CITS4403** (SEM-2) **Lecture_Tutorial** RBST: [G16] **Wks** 30-35, 37, 40-42				
10:00 AM					
11:00 AM					
12:00 PM					
1:00 PM					
2:00 PM		**CITS4403** (SEM-2) **Laboratory** CSSE: [201] **Wks** 30-35, 37-42			
3:00 PM					
4:00 PM				**CITS4403** (SEM-2) **Laboratory** ENCM: [207A] **Wks** 30-35, 37-42	
5:00 PM					
6:00 PM					

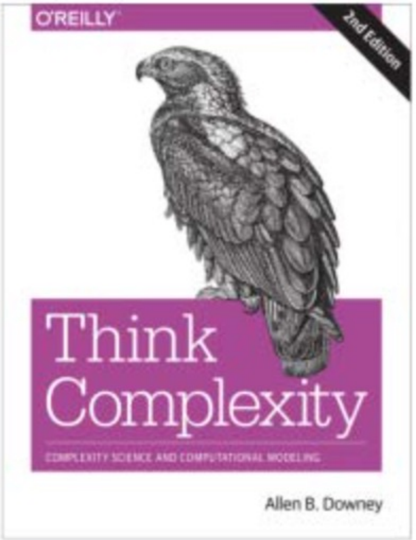
Lab starts in Week 2

Recommended Textbook:

> Downey, A. (2018). Think complexity: complexity science and computational modeling. " O'Reilly Media, Inc.".

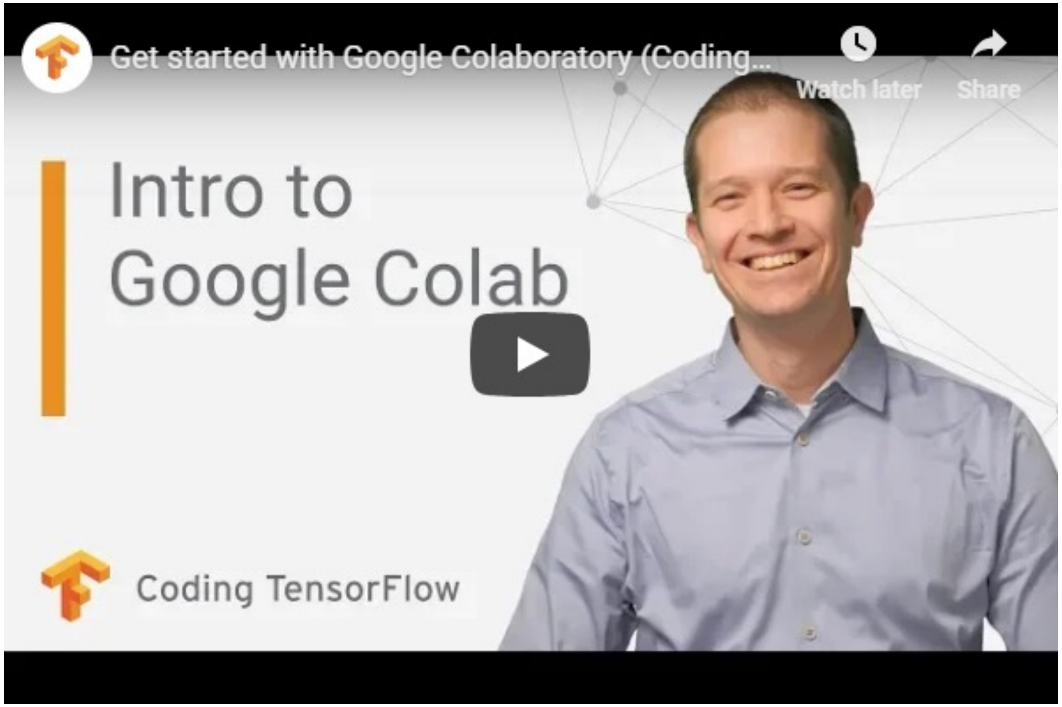
You can download the PDF from:

https://greenteapress.com/complexity2/thinkcomplexity2.pdf



We will use Google Colab for all Lecture and Lab relevant code. But you're allowed to use other IDE if you prefer.

Colaboratory is a free Jupyter notebook environment that requires no setup and runs entirely in the cloud. With Colaboratory you can write and execute code, save and share your analyses, and access powerful computing resources, all for free from your browser.



https://colab.research.google.com/notebooks/intro.ipynb

You are expected to know Python:

- By that, I mean you are a confident in python programming
- You are expected to be able to read the code, understand the code and implement the algorithms
- We will go through code together in some lectures
- Project will involve programming
- There will be **NO NON-programming option** for project
- There will be coding question in exams

STAFF

Unit Coordinator & Lecturer

- siwen.luo@uwa.edu.au
- No fixed consultation hour; please arrange a time with me by email.
- For any questions related to the course, e.g. course contents and admin issues, please contact the unit coordinator directly by email.
- Please put [CITS4403] in the title of your email

Lab Facilitators

- I will introduce them in your first lab.

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Special Consideration

What do you do if you get sick during semester?

Please check the UWA Special Consideration Webpage:

https://www.uwa.edu.au/students/my-course/exams-assessments-and-results/special-consideration

You need to share your special consideration approval to the Unit Coordinator within **3 days**.

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What is Computational Modelling?

Computational Modelling is the use of computers to *simulate and study complex systems* using mathematics, physics and computer science. It allows scientists to conduct thousands of simulated experiments by computer.

Computational Model

Simulation

Complex Systems

Computational Model and Simulation

A **computational model** contains numerous variables that characterize the system being studied.

Simulation is done by adjusting the variables alone or in combination and observing the outcomes.

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Computational model captures the behaviour of the complex system being modelled.

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Simulation is done by adjusting the variables alone or in combination and observing the outcomes.

Simulation is the process of running a computational model.

Computational Model and Simulation

Build a simulation? ✗

Computational Model and Simulation

Build a simulation? ✗

Build a model or Build a simulator ✓

Run the model or Build a simulation ✓

We don’t run Simulation just once in actual experiments!

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What is complex system?

A **system** is a group of interacting or interrelated **elements** that act according to a set of rules to form a unified whole.

A **complex system** are composed of many **components** (or **systems**) which may interact with each other.

3 Complex Systems

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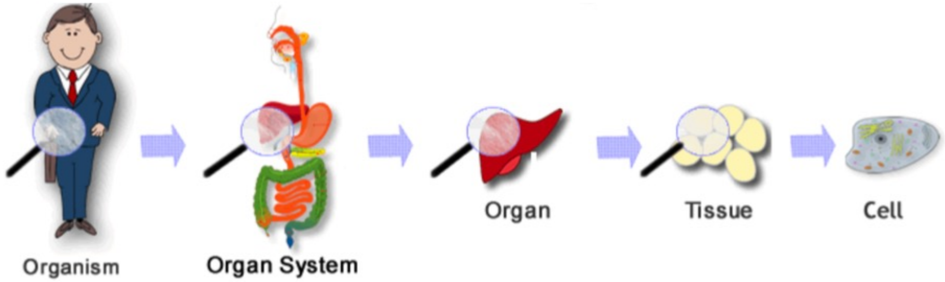
These two concepts look quite similar? 🤔

A complex system is just a special category of system, with some special features.

Complex Systems

A **complex system** are composed of many **components** (or **systems**) which may interact with each other.

E.g. people are made up of organ systems, which are made up of organs, which are made up of tissues, which are made up cells.



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Complex Systems

A **complex system** are composed of many **components** (or **systems**) which may interact with each other.

E.g. Local economy is a part of national economy, which in turn is a part of global economy. Each is interconnected and independent from others.

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Complex Systems

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Complex Systems

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Complex System Features

Interactions

A **complex system** are composed of many **components** (or **systems**) which may **interact** with each other.

Components that **interact** in multiple ways among **each other** and potentially with their **environment** too. These components form networks of interactions.

Interactions may generate novel information that make it difficult to study components in isolation or to completely predict their future.

The main challenge of studying complex system is not only to see the parts and their connections but also to understand how these connections give rise to the whole.

Complex System Features

Emergence

The main challenge of studying complex system is not only to see the parts and their connections but also to understand **how these connections give rise to the whole.**

In **simple systems**, the properties of the whole can be understood or predicted from the addition or aggregation of its components.

In **complex systems**, however, the properties of the whole often cannot be understood or predicted from the knowledge of its components.

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Emergence

The main challenge of studying complex system is not only to see the parts and their connections but also to understand **how these connections give rise to the whole.**

The whole is more than the sum of its parts.

Phenomenon of Emergence
Interaction between components generate novel information and exhibit non-trivial collective structures and behaviors at larger scales.

https://www.youtube.com/watch?v=16W7c0mb-rE

Complex System Features

Dynamic

Complex systems tend to change their **states** dynamically, often showing unpredictable long-term behaviour.

> **state**: sets of variables that best characterize the system.

Complex systems are typically **non-linear,** changing at different rates depending on their states and their environment.

Some systems are chaotic, extremely sensitive to small perturbations and unpredictable in the long run, showing the so-called butterfly effect.
E.g. weather constantly changing in unpredictable ways.

Complex System Features

Self-Organization

Complex systems may self-organize to produce non-trivial patterns spontaneously.

Interactions between components of a complex system may produce a global pattern or behaviour, **without** central or external controller. The “control” of a self-organizing system is distributed across components and integrated through their **interactions**.

As the system becomes more organized by this process, new interaction patterns may emerge over time, potentially leading to the production of greater complexity.
E.g. single cell dividing and self-organizing into complex shape of an organism.

3 Complex System Features

Adaptation

Complex systems may **adapt** and **evolve**.

Complex systems are often active and responding to the environment. When the components are damaged or removed, these systems are often able to adapt and recover their previous functionality, and sometimes they become even better than before.

E.g. an immune system continuously learning about pathogens

Interdisciplinarity

Complex systems appear in all scientific and professional domains, including *physics, biology, ecology, social sciences, finance, business, management, politics, psychology, anthropology, medicine, engineering, information technology, and more.*

Many systems in different domains display phenomena with common underlying features that can be described using the same scientific models.

3 Complex System Features

E.g. *Tracking infectious diseases in medical science and study.*

Computational models are being used to track infectious diseases in populations, identify the most effective interventions, and monitor and adjust interventions to reduce the spread of disease.

E.g. *Physics simulation*

In 2022, researchers build a black hole simulation by modelling a single-file chain of atoms to create the event horizon of a black hole.

E.g. Traffic Jams:
https://www.complexity-explorables.org/explorables/berlin-8-am/

E.g. Bird flocks:
https://www.complexity-explorables.org/slides/flockn-roll/

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Complexity Science – science for complex systems.

It is a *gradual shift* in the criteria models are judged by, and in the kinds of models that are considered acceptable.

Classical Science

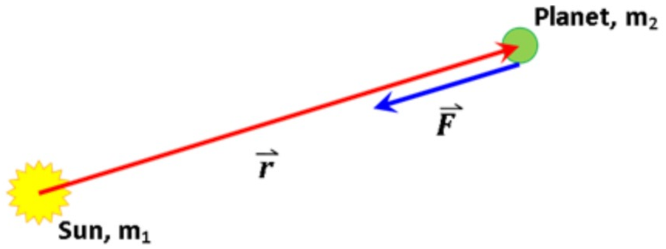
Why planetary orbits are elliptical?

The notion that planets revolve about the sun in elliptical orbits was found empirically by Johannes Kepler. Later, the fundamental principles elucidated by Isaac **Newton** provided a firm theoretical basis for understanding such orbits.

By taking derivatives over **Newton's second law** of motion F= ma, the expression for the gravitational force, F, is written in terms of the planet's radial position, r:

$$\vec{F} = \frac{-G\, m_1\, m_2}{r^2}\,\hat{r},$$

where m_1 is the mass of the sun,
m_2 is the mass of the planet,
r is the radial distance between the sun and planet,
G is the universal gravitational constant,
$\hat{r}$ is the unit vector in the radial direction.



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Complexity Science

Why Detroit is racially segregated?

The Schelling model of the city is an array of cells where each cell represents a house. The houses are occupied by two kinds of "**agents**", labelled **red** and **blue**, in roughly equal numbers. About 10% of the houses are empty.

At any point in time, an agent might be happy or unhappy, depending on the other agents in the neighbourhood. In one version of the model, agents are happy if they have at least two neighbours like themselves, and unhappy if they have one or zero.

The simulation proceeds by choosing an agent at **random** and checking to see whether it is happy. If so, nothing happens; if not, the agent chooses one of the unoccupied cells at **random** and moves.

Complexity Science vs. Classical Science

Classical models tend to be **law-based**, expressed in the form of **equations**, and solved by **mathematical derivation.**

Complexity models are **rule-based**, expressed as simple computation instead of mathematical derivation, and are simulated not mathematical analyzed.

Classical Science vs. Complexity Science

Classical Science	**Complexity Science**
Equation-based	**Simulation-based**
Analysis	**Computation**
Continuous	**Discrete**
Deterministic	**Stochastic**
One/Two components	**Many components**
Homogeneous	**Heterogeneous**
Predictive	**Explanatory**
Reductionism	**Holism**
Isolation	**Interaction**

5 NEXT WEEK PREVIEW…

1. Graphs
   - Different graph types
2. Regular Graph vs Random Graph
3. Erdos Renyi Graphs and Implementation