Simulation, Analysis, and Validation of Computational Models

Course Organisation

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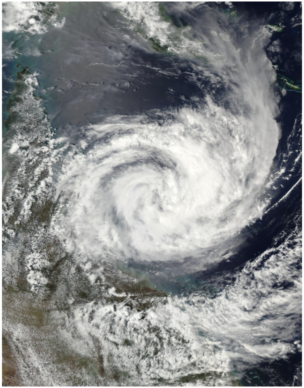
Motivation

Challenges of the 21st Century*: Predict, understand, and control complex dynamical systems

- Climate change, flood risk, natural hazards
- Biodiversity, deforestation, over-fishing
- Sustainability, resources, pollution
- Economy, cost of living
- Population growth, urbanisation, migration
- Pandemics, global health
- Energy distribution, technology, recycling



By MODIS imagery from NASA's Aqua Satellite - EOSDIS Worldview, CC BY-SA 4.0

*This is not a complete list, some challenges are not less serious, but less connected to this course.

Course name

- Simulation, Analysis, and Validation of Computational Models
  - **Simulation**: What can we learn from a simulation about the *world*?
  - **Analysis**: How can we use simulations most efficiently to improve our understanding of the *world*?
  - **Validation**: To what extent we can trust the simulation?
  - **Computational Models**: What are we are going to work with?
- Alternative names of this course
  - *Dynamics in Action*
  - *Scientific computing*
  - *Physics-Informed Neural Networks (PINN)*

Lectures

- Lectures (10 main units (examinable),
  3 supplementary units ("examinable"), plus a few bonus units (non-examinable*)
- Slides are available from the day before the lecture.
- Lecture recordings will available with probability > 0.8

*Edinburgh marking schemes applies

Workshops

- Weeks 4 to 6
- Content:
    - Practical exercises
    - Prerequisites: Python
    - Preparation of coursework
    - Discussion of coursework
- Follow by weekly office hour

Coursework Assignment

- From 10th October to 21th November (6 weeks)
- In the first week (10/10 - 17/10) a preliminary version will be available, which is open to discussion.
- Unmarked intermediate report can be submitted in the first week of October
- Includes
  - programming tasks (python)
  - testing a few variants of your program
  - statistical analysis
  - scenario evaluation
  - graphical representation
  - report
- Worth 30% of course mark

Quizzes

- Reachable in Learn $\rightarrow$ Assessment
- Not marked (unlimited attempts)
- Instant automatic feedback
- Multiple choice questions which are meant to be easy
- 5 quizzes of 10 questions each
- Starting in second week, one by one added and available for the rest of term

Exam

- December diet
- 70% of course mark
- Questions
  - A set of simple problems, straight-forwardly answerable questions (similar to the quiz questions, but not MCQs)
  - Two options each of which includes
    - a theoretical question
    - an application-oriented question
- No past papers available, but a mock exam will be arranged as a take-home task in week 10/11, with general feedback / sample solutions in week 11/12, depending on the date of exam which will be known around the end of October and on similarity of the mock questions and the real exam questions, and whether there are any responses to the mock exam.

“What do we need to know for the exam?”

- Understanding of basic forms of main approaches, concepts and methods
- Case studies will not be checked, but can help to design a qualitative solution for other cases
- ‘Open book’ (a few sheets a paper can be taken into the exam hall)
- Revision meeting in week 11/12

Prerequisites

- Programming: Python will be used in tutorials and in coursework
- It will be useful to revise some maths topics:
  - linear algebra: N-dim. space, hyperplanes, eigenvalues, eigenvectors
  - geometry: generalisation of spheres and cubes to higher dimensions
  - calculus: convergence, gradients, extremal values of a function
  - probability and statistics: correlation matrices, Bayes' rule, law of large numbers
- Computing: Algorithms, data structures, concurrency
- Physics, engineering, finance : This courses is about modeling and simulation, so it cannot hurt to have a good understanding of one or more of the target.

Overview

wk	Tuesday	Friday	CW	workshops	Quiz
1	Intro	Lect. 1			⇓
2	Lect. 2	Lect. 3			1
3	Lect. 4	Lect. 5			⇓
4	Lect. 6	CW	⇓	W1	2
5	Lect. 7	Lect. 8	⇓	W2	⇓
6	Case 1	Case 2	⇓	W3	3
7	Case 3	Feedback	⇓	Drop-in	⇓
8	Lect. 9	Lect. 10	⇓	Drop-in	4
9	Bonus 1	Bonus 2	⇓	Drop-in	⇓
10	Bonus 3	Gen. FB			5
11	Revision	[Indiv. FB]			
T	50'	50'	$\leq$20h	100'	20'
Σ	8h	8h	$\leq$20h	6h	2h

Topics

- Intro: Simulation vs. modelling
- Lecture 1: Principles of systems science, computational syst.
- Lecture 2: Monte Carlo, Markov chain (Ch 1, 2)
- Lecture 3: Quantitative modelling, causality (Ch 4)
- Lecture 4: Parameter estimation, sensitivity analysis, control
- Lecture 5: Phase transitions, bifurcations, uncertainty (Ch 5)
- Lecture 6: System modelling and engineering
- Lecture 7: Multi-Agent Systems, governance, society (Ch 7)
- Lecture 8: Spreading of diseases, misinformation (Ch 8, 9)
- Case study 1: Robotics: (Ch 3)
- Case study 2: Finance: Finance: (Ch 6)
- Case study 3: Weather, climate
- Lecture 9: Testing, validation, verification, confidence
- Lecture 10: Explainability, scaling, complexity, heterogeneity
- Bonus: PINN and current research

Literature

- Rongpeng Li & Aiichiro Nakano (2022) Simulation with Python: Develop simulation and modeling in natural sciences, engineering, and social sciences. Apress (Springer). [accessible]
- George E. Mobus & Michael C. Kalton (2015) Principles of systems science. Springer. [classical]
- George E. Mobus (2022) Systems science: Theory, analysis, modeling, and design. Springer. [“philosophical”]
- Hugues Goosse (2015) Climate system dynamics and modelling. Cambridge University Press. [specialised]
- Bilash Kanti Bala, Fatimah Mohamed Arshad, Kusairi Mohd Noh (2017) System dynamics modelling and simulation. Springer [case studies]
- Research papers recommended with context (not required)

Relation to other courses

Introduction to the Theory of
❧ Natural Computing ☙

Modelling of Systems for Sustainability (MOSS)

- Excellent prerequisite, but not required
- Quantitative modelling
- Computational expertise
- Wider scope and application to various fields

Next topics

- Simulation vs. modelling
- Systems thinking
- Linearity and non-linearity