MODULE TITLE	**Computational Modelling and Simulation**	**CREDIT VALUE**	**30**
MODULE CODE	**MTHM607**	**MODULE CONVENER**	**Dr Markus Mueller (Coordinator)**

DURATION: TERM	**1**	**2**	**3**
DURATION: WEEKS	**11**		

Number of Students Taking Module (anticipated)	**20**

DESCRIPTION - summary of the module content

The complexity of mathematical and computational models describing most natural and man-made systems necessitates modern numerical methods and analysis of computer simulations. In this module you will develop computational modelling and simulation skills within a context of essential, high-value applications, using state-of-the-art scientific computing software. The module will be problem focussed, taking real-world examples, and using these to inform your understanding and appreciation of the underlying modelling and simulation methods. The module will draw from a range of topics: large partial differential equation-based modelling of flows and fields; computer-aided systems analysis; stochastic systems; and approaches to modelling the environment and natural systems. You will communicate your models and findings to your peers and for assessment through reports, presentations and other digital media.

AIMS - intentions of the module

This module intends to introduce students to modern numerical algorithms design and computational techniques for mathematical modelling and simulation. You will explore modelling from first principles and the design and implementation of computational models using MATLAB or Python or similar high-level languages. The module follows a two-step learning process: (1) you are introduced to a modelling approach, and (2) you develop the approach within a substantive application.

INTENDED LEARNING OUTCOMES (ILOs) (see assessment section below for how ILOs will be assessed)

On successful completion of this module **you should be able to**:

Module Specific Skills and Knowledge:
1 Formulate mathematical models from first principles;
2 Design modern numerical algorithms for mathematical modelling;
3 Use your programming skills in MATLAB or Python or similar high-level language to model challenging mathematical problems;

Discipline Specific Skills and Knowledge:
4 Tackle a wide range of applied mathematical problems using modern numerical methods;
5 Model real-world problems and understand the principles underlying the techniques and when they are applicable;

Personal and Key Transferable/ Employment Skills and Knowledge:
6 Show enhanced modelling, problem-solving and computing skills, and acquired tools that are widely used in mathematical modelling and simulation;
7 Communicate the value of modelling and simulation to a range of end users in life and environmental sciences, or energy engineering.

SYLLABUS PLAN - summary of the structure and academic content of the module

The aim of the module is to make sure the approaches are modern and current and so the specific modelling approaches may vary over time. Each modelling approach will be covered in blocks of intense learning and creating, in which an approach is introduced and then applied in mini-project based work. A selection of topics from the following list will be covered:

Fluids and flows
Part 1: Revision of numerical methods for Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs);
Part 2: Mathematical modelling and simulation of partial differential equations in fluid mechanics, fluid sloshing problem in Lagrangian particle-path and Eulerian coordinates;
Part 3: Introduction to Simulating Hamiltonian Systems: geometric and structure-preserving numerical methods; Stormer-Verlet and Shake-Rattle algorithms; Poisson-bracket discretisation;
Part 4: Symplectic integration and computational modelling of rigid-body dynamics, and mathematical fluid mechanics problems;

Computer-aided systems analysis
Part 1: Dynamical systems modelling and simulation: Modelling principles for natural and engineering systems; Equilibrium states analysis; Stability analysis; Applications from population ecology, resource analysis, engineering;
Part 2: Systems dynamics modelling and simulation: Levels and rates in systems dynamics; Causal and feedback loops; Diagrammatic process models; Applications from socio-economic systems, earth systems;
Part 3: Numerical methods: Finite element/finite difference/finite volume techniques;

Stochastic systems
Part 1: Markov processes and Markov chain modelling; Discrete-time Markov chains; Continuous-time Markov chains; Properties of Markov chains; Random walks;
Part 2: Time-series analysis and signal processing; Moving average models; Auto-regressive models; ARMA; ARIMA;
Part 3: Limit theorems; Central limit theorem; Law of large numbers; Ergodic theorems;

Populations and patterns
Part 1: Population modelling; Single species models; Interactive population models; Meta-population models; Spatio-temporal population models;
Part 2: Collective behaviour and movement dynamics; Agent-based modelling;
Part 3: Dynamics of Infectious Diseases; Compartmental models; Epidemiological networks and spatial epidemiology;
Part 4: Pattern formation; Reaction diffusion systems; Chemotaxis.

LEARNING AND TEACHING

LEARNING ACTIVITIES AND TEACHING METHODS (given in hours of study time)

Scheduled Learning & Teaching Activities	60.00	**Guided Independent Study**	240.00	**Placement / Study Abroad**	

DETAILS OF LEARNING ACTIVITIES AND TEACHING METHODS

Category	Hours of study time	Description
Scheduled Learning and Teaching Activities	24	Lectures and tutorials
Scheduled Learning and Teaching Activities	6	Student-led presentations
Scheduled Learning and Teaching Activities	30	Computer-based modelling workshops
Guided Independent Study	260	Lecture and assessment preparation, computing, wider reading

ASSESSMENT

FORMATIVE ASSESSMENT - for feedback and development purposes; does not count towards module grade

Form of Assessment	Size of Assessment (e.g. duration/length)	ILOs Assessed	Feedback Method
Exercises and/or mini-projects	3 x 5 hours	1-5, 7	Oral

SUMMATIVE ASSESSMENT (% of credit)

Coursework	100	Written Exams	0	Practical Exams	0

DETAILS OF SUMMATIVE ASSESSMENT

Form of Assessment	% of Credit	Size of Assessment (e.g. duration/length)	ILOs Assessed	Feedback Method
Coursework portfolio	60	Three project- or exercise-based reports (3 x 1,500 words or equivalent), each relating to a module topic	1-7	Written and verbal
Model design and demonstration	40	Design and implementation of a complex computational model (>500 lines of code and documentation) and its demonstration	1-3, 5, 6	Written and verbal

DETAILS OF RE-ASSESSMENT (where required by referral or deferral)

Original Form of Assessment	Form of Re-assessment	ILOs Re-assessed	Time Scale for Re-assessment
Coursework portfolio	Coursework (100%)	1-7	To be agreed by consequences of failure meeting
Model design and demonstration	Coursework (100%)	1-3, 5, 6	To be agreed by consequences of failure meeting

RE-ASSESSMENT NOTES

Deferral – if you miss an assessment for certificated reasons judged acceptable by the Mitigation Committee, you will normally be either deferred in the assessment or an extension may be granted. The mark given for a re-assessment taken as a result of deferral will not be capped and will be treated as it would be if it were your first attempt at the assessment.

Referral – if you have failed the module overall (i.e. a final overall module mark of less than 50%) you will be required to resubmit the original assessment as necessary. The mark given for a re-assessment taken as a result of referral will be capped at 50%.

RESOURCES

INDICATIVE LEARNING RESOURCES - The following list is offered as an indication of the type & level of information that you are expected to consult. Further guidance will be provided by the Module Convener

Web-based and electronic resources:

• **ELE -** http://vle.exeter.ac.uk/

Other resources:

• N.A.

Reading list for this module:

Type	Author	Title	Edition	Publisher	Year	ISBN	Search
Set	Curran, Mary Ann	Life Cycle Assessment Handbook: A Guide for Environmentally Sustainable Products		Wiley	2012	978-1-118-09972-8	[Library]
Set	Forrester, J.W.	Urban Dynamics		Pegasus Communications	1969	978-1-883823-39-9	[Library]
Set	Hairer, E., Lubich, C. & Wanner, G.	Geometric Numerical Integration		Springer	2002	978-3-540-30666-5	[Library]
Set	Jones P.W. and Smith P.	Stochastic Processes: methods and applications		Arnold	2001	000-0-340-80654-0	[Library]
Set	Leimkuhler, B. & Reich, S.	Simulating Hamiltonian Dynamics		Cambridge University Press	2004	978-0-511-61411-8	[Library]
Set	Meadows, D.H.	Limits to Growth		University Books	1972	978-0-87663-165-2	[Library]
Set	Meadows, D.H., Randers, J. & Meadows, D.L.	The Limits to Growth: The 30-year Update		Hill & Wang	2006	978-0809029570	[Library]
Set	Morecroft, J.	Strategic Modelling and Business Dynamics: A Feedback Systems Approach		Wiley	2007	978-0-470-01286-4	[Library]
Set	Norris, J. R.	Markov Chains		Cambridge University Press	1998	978-0521633963	[Library]
Set	Pastor, J.	Mathematical Ecology of Populations and Ecosystems		Wiley	2008	9781405177955	[Library]
Set	Sorensen, Bent	Life-Cycle Analysis of Energy Systems: From Methodology to Applications		Royal Society of Chemistry	2011	978-1-84973-145-4	[Library]

CREDIT VALUE	30	ECTS VALUE	15

PRE-REQUISITE MODULES	None
CO-REQUISITE MODULES	None

NQF LEVEL (FHEQ)	7	AVAILABLE AS DISTANCE LEARNING	No
ORIGIN DATE	Wednesday 16 December 2020	LAST REVISION DATE	Thursday 26 January 2023

KEY WORDS SEARCH	First principles; Mathematical modelling; Scientific programming; Simulation; Computation; Ecological dynamics; Environmental modelling