ES98D-15 Particle-based modelling

24/25

Department
School of Engineering
Level
Taught Postgraduate Level
Module leader
Albert Bartok-Partay
Credit value
15
Module duration
10 weeks
Assessment
60% coursework, 40% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

Particle-based simulations are used to study processes from the microscopic to astronomic scales. Examples include atomic and colloidal systems, biological cells, epidemiology, crowds, self-driving cars or astronomical objects. This module will introduce the statistical mechanics foundations of modelling, and will cover methods such as molecular dynamics, Monte Carlo and lattice based simulations. Problem focussed workshop sessions will illustrate the use of software tools for specific groups of models. Case studies by guest lecturers will provide further insight into applications.

Module aims

To introduce the theory of particle- and agent-based simulation techniques and provide practical experience in specific application areas.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

This module will introduce particle based simulation for students studying for the MSc in Predictive Modelling. A theoretical discussion of the statistical mechanics basics will be followed by

applications of these principles in different domains, with examples from guest lecturers changing from year to year and including topics such as:

- atomistic simulations for materials and molecular modelling
- lattice models, such as the Ising model to illustrate statistical physics concepts
- coarse grain models of colloidal particles or biological cells
- simulations for active matter, such as flocking or crowd dynamics
- agent based modelling, such as epidemiology or self-driving cars
- astronomical modelling.

Learning outcomes

By the end of the module, students should be able to:

- Interpret the statistical mechanics of particles
- Demonstrate substantial familiarity with application areas of particle-based simulations
- Develop software tools to model assemblies of entities
- Evaluate the uncertainty of simulation results
- Design computational experiments to predict quantities of interest

Indicative reading list

Research articles in the field will complement the books.

View reading list on Talis Aspire

Subject specific skills

To understand statistical mechanics and its applications in different scientific and engineering domains.
To design, perform and analyse simulation experiments, quantifying the uncertainty in the results.
To appreciate capabilities and limitations of simulation studies.

Transferable skills

Ability to work with diverse software environments.
Ability to create automated, reproducible and robust workflows.
Problem solving, logical reasoning.

Study

Study time

Type	Required
Lectures	12 sessions of 2 hours (16%)
Supervised practical classes	5 sessions of 3 hours (10%)
Private study	111 hours (74%)
Total	150 hours

Private study description

Further reading on background, revision.

Costs

No further costs have been identified for this module.

Assessment

You must pass all assessment components to pass the module.

Assessment group D1

	Weighting	Study time
Workshop assignments	60%	

Students will submit reports on each of the workshop assignments. The assessed work will be 1-page reports (or equivalent amount of computer-based notebooks) consisting of original code, graphs and interpretation.

Viva Voce Exam	40%	

Students will be examined on the core topics covered in the lectures and the critical analysis of a research paper. The exams will be conducted by two members of staff, lasting 25 minutes.

Feedback on assessment

Written individual and group feedback on workshop reports
Discussion during the viva examination
Written summary of viva performance

Past exam papers for ES98D

Availability

Courses

This module is Core optional for:

- Year 1 of TESA-H1B1 Postgraduate Taught Predictive Modelling and Scientific Computing