

159.240 Computational Science

Important Information

Summer School 2014

159.240 Computational Science

Some important details:

- 159.240 is internal, 15-credit
- Paper coordinator: Dr Alwyn Husselmann
 - Room 3.05 in IIMS bldg
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- **Aim:** A study of the essentials of scientific programming.

159.240 Computational Science

- There are several assignments
- You are expected to know how to write, compile and debug C/C++ programs!
- Prerequisites: 159.101, 160.1xx
 - If you have not passed either of these courses, you need to see the lecturer ASAP

Learning Outcomes

- Formulate the programming requirements of a scientific computation
- Discuss the possible effects of error propagation, random number generation and selection of numerical algorithms on the accuracy and efficiency of computational software.
- Describe and review the use of evolutionary algorithms and related techniques in the construction of computer simulations and models.
- Program, test and run a numerical simulation experiment and analyse its results and implications.

Stream

- Slides and course material are made available on Stream
- Generally, assignment skeleton code is provided on Stream
- Assignments are submitted through Stream

Marks

- Assessment weightings (45%):
 - Assignment 1 – 10%
 - Assignment 2 – 10%
 - Assignment 3 – 15%
 - Assignment 4 – 10%
- Final exam – 55%

Lectures

3 hours per week, optional lab time

- Monday 9am-10am QA4 Lecture
- Wednesday 10am-12noon QA4 Lecture
- Friday 10am – 12noon CLQB4 Lab Time
 - Optional, attended from 10-11
- Please come to lectures, it will be difficult to pass the course without them.

Christmas Timing etc

- Christmas break from 24 December to 2 January
- But **no lecture** on 22 December

Broad Topics Covered

- Random numbers
- Computational errors
- Complex Systems and Simulations
- Agent-based Modelling
- Global Optimisation

Recommended Reading

- No prescribed textbook
- Lots of material online

Suggested (***not prescribed***)

- *Introduction to Computational Science*
 - Shiflet & Shiflet, 2014

Assignments

- C/C++ assignments, done at home or at university labs (note: mostly Win32)
 - Assignments **must** compile and run in labs
- Submit your assignments via Stream, not via emails
- You can work in groups of up to 3 students
 - You **MUST** ensure all names and ID numbers appear at the top of the file as a comment.

Assignments

- Assignment 1 (10 marks)
 - Levy-flight simulation, random numbers and simulation basics
- Assignment 2 (10 marks)
 - Monte Carlo simulation, simple method to calculate Pi
- Assignment 3 (15 marks)
 - Flocking simulation, modelling bird flocking behaviour
- Assignment 4 (10 marks)
 - Particle Swarm Optimiser (optimisation)

Due dates

- Please submit by the due date
- 1 mark off per day late...
- If late, it may be some time before marking occurs
- Assignments can only be submitted once, remarking cannot be done

Lecture Outline

- Simulations and Randomness
 - Brief introduction on simulations
 - Random numbers
 - Random number distributions
 - Programming random number generators
 - Random walks

Assignment 1: Levy flight simulation

Lecture Outline

- Computational errors and good practices
 - Overview of errors in models/simulations
 - Rounding errors
 - Significant figures
 - Word sizes
 - Conversion errors
 - Etc
 - Coding practices

Lecture Outline

- Programming Simulations
 - Basics
 - Visualisation
 - Linear algebra
 - Dealing with collected data

Assignment 2: Monte Carlo simulation

Lecture Outline

- Agent-based modelling
 - Overview
 - Programming ABMs
 - Principles
 - Examples

Assignment 3: Flocking simulation

Lecture Outline

- Global optimisation
 - Particle-based optimisers
 - Bio-inspired optimisation
 - Particle Swarm Optimisers
 - Firefly Algorithms
 - Evolutionary Algorithms
 - Genetic Algorithms
- Assignment 4: Particle Swarm Optimiser