Scientific Computing and Data Science

Title	Scientific Computing and Data Science
Semester	F2023
Master programme in	Mathematical Bioscience / Physics and Scientific Modelling
Type of activity	Course
Teaching language	English
Study regulation	Read about the Master Programme and find the Study Regulations at [ruc.dk](ruc.dk) Læs mere om uddannelsen og find din studieordning på [ruc.dk](ruc.dk)

REGISTRATION AND STUDY ADMINISTRATIVE

Registration	Sign up for study activities at stads selvbetjening within the announced registration period, as you can see on the Studyadministration homepage. When signing up for study activities, please be aware of potential conflicts between study activities or exam dates. The planning of activities at Roskilde University is based on the recommended study programs which do not overlap. However, if you choose optional courses and/or study plans that goes beyond the recommended study programs, an overlap of lectures or exam dates may occur depending on which courses you choose.
Number of participants	
ECTS	10
Responsible for the activity	Thomas Schrøder (tbs@ruc.dk)
Head of study	Studieleder for Fysik (fys-sl@ruc.dk)
Teachers	
Study administration	INM Registration & Exams (inm-exams@ruc.dk)
Exam code(s)	U60190

ACADEMIC CONTENT

Overall objective	To give the student experience in choosing and applying the methods of Scientific Computing and Data Science to new problems and to give the

	student an overview of methods associated with: - Scientific Computing, i.e., the use of computers and applied math to generate data from models by numerical methods and/or simulation. - Data Science, i.e., the use of computers, models, and applied math to gain insight from data.
Detailed description of content	The aim of the course is to give the student experience in choosing and applying methods of Scientific Computing and Data Science to (for the student) new problems and to give the student an overview of methods associated with the two subjects: ● Scientific Computing, i.e., the use of computers and applied math to generate data from models by numerical methods and/or simulation. In the first mini-project students will work in groups to implement the so-called molecular-dynamics method in Python. This includes the relevant testing and interpretation of results. ● Data Science, i.e., the use of computers, models, and applied math to gain insight from data. In the second mini-project, students will work in groups to apply data science methods to scientific data of their own choice, and report their conclusions in a convincing way. In the third and final mini-projct students groups can choose between the two subjects (Scientific Computing and Data Science) or a combination thereof. If a single subject is chosen, the mini-project must include a discussion of how the other subject could be involved.
Course material and Reading list	To be specified on moodle
Overall plan and expected work effort	10 ECTS course ● Reading course material and problem solving at home: 70 hrs ● Discussion and problem solving in class: 30 hrs ● Working on mini-projects at home: 100 hrs ● Working on mini-projects in class: 60 hrs ● Exam preparation: 9 hrs ● Exam: 1 hours - **Total 270 hrs**
Format	
Evaluation and feedback	The course includes formative evaluation based on dialogue between the students and the teacher(s). Students are expected to provide constructive critique, feedback and viewpoints during the course if it is needed for the course to have better quality. Every other year at the end of the course, there will also be an evaluation through a questionnaire in SurveyXact. The Study Board will handle all evaluations along with any comments from the course responsible teacher. Furthermore, students can, in accordance with RUCs 'feel free to state your views' strategy through their representatives at the study board, send evaluations, comments or insights form the course to the study board during or after the course.
Programme	Theme 1: Scientific Computing. First mini-project: Molecular Dynamics

Theme 2: Data Science. Second mini-project: Application of data science methods to scientific data

Theme 3: Third mini-project: Scientific computing and/or data science

ASSESSMENT

Overall learning outcomes

After completing the course the students will be able to

- demonstrate an overview of methods in Scientific Computing and Data Science.
- choose methods in Scientific Computing and Data Science relevant for a given problem.
- independently learn about methods in Scientific Computing and Data Science on an advanced level.
- apply methods in Scientific Computing and Data Science to a new problem. This includes the relevant programming, testing, and interpretation of results.

Form of examination

Individual oral exam based on a portfolio.

The character limit of the portfolio is 1,200-120,000 characters, including spaces. Examples of written products are exercise responses, talking points for presentations, written feedback, reflections, written assignments. The preparation of the products may be subject to time limits.
The character limits include the cover, table of contents, bibliography, figures and other illustrations, but exclude any appendices.

Time allowed for exam including time used for assessment: 30 minutes. The assessment is an assessment of the oral examination. The written product(s) is not part of the assessment.

Permitted support and preparation materials for the oral exam: All.

Assessment: 7-point grading scale.
Moderation: Internal co-assessor

Form of Re-examination

Samme som ordinær eksamen / same form as ordinary exam

Type of examination in special cases

Examination and assessment criteria

The students produce a portefolio consisting of 3 mini-projects. All 3 can be handed-in for review by the teacher.

At the exam the student makes a presentation of the third mini-project. The presentation may be interrupted by clarifying questions and the presentation will be followed by a discussion and questioning with in the curriculum of the course.

Students will be assessed by their ability to:

- apply methods in Scientific Computing and Data Science to a new problem. This includes the relevant programming, testing, and interpretation of results.

- argue for choosing specific methods in Scientific Computing and Data Science relevant for a given problem.
- demonstrate that they have independently learnt about methods in Scientific Computing and Data Science on an advanced level.

The assessment of the oral exam is based on the student's ability to meet the criteria mentioned above and their ability to

- clearly present and communicate the scientific content of the portfolio
- engage in a scientific dialogue and discussion with the assessor and co assessor

Furthermore, whether the performance meets all formal requirements in regard to both for the written og oral exam

Exam code(s)	Exam code(s) : U60190

Course days:

Hold: 1

Scientific Computing and Data Science (MathBio)

time	07-02-2023 08:15 til 07-02-2023 12:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio) - please note room in 12.1 due to RUC Open House

time	09-02-2023 12:15 til 09-02-2023 14:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	12.1-073 - teorilokale i 12.1 (30)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	14-02-2023 08:15 til 14-02-2023 12:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.2-064 - pc lokale (40)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	16-02-2023 12:15 til 16-02-2023 14:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	21-02-2023 08:15 til 21-02-2023 12:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	23-02-2023 12:15 til 23-02-2023 14:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	28-02-2023 08:15 til 28-02-2023 12:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.2-064 - pc lokale (40)

Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	02-03-2023 12:15 til 02-03-2023 14:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	07-03-2023 08:15 til 07-03-2023 12:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.2-064 - pc lokale (40)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	09-03-2023 14:15 til 09-03-2023 16:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	14-03-2023 08:15 til 14-03-2023 12:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.2-064 - pc lokale (40)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	16-03-2023 14:15 til 16-03-2023 16:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	21-03-2023 08:15 til 21-03-2023 12:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.2-064 - pc lokale (40)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	23-03-2023 14:15 til 23-03-2023 16:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	28-03-2023 10:15 til 28-03-2023 12:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.2-064 - pc lokale (40)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	04-04-2023 10:15 til 04-04-2023 12:00
location	27.2-064 - pc lokale (40)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   11-04-2023 10:15 til
            11-04-2023 12:00

location   27.2-064 - pc lokale (40)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   14-04-2023 08:15 til
            14-04-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   18-04-2023 10:15 til
            18-04-2023 12:00

location   27.2-064 - pc lokale (40)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   21-04-2023 08:15 til
            21-04-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   25-04-2023 10:15 til
            25-04-2023 12:00

location   27.2-064 - pc lokale (40)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	28-04-2023 08:15 til 28-04-2023 12:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	02-05-2023 10:15 til 02-05-2023 12:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	04-05-2023 12:15 til 04-05-2023 16:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	09-05-2023 10:15 til 09-05-2023 12:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time	12-05-2023 08:15 til 12-05-2023 12:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   16-05-2023 10:15 til
        16-05-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   19-05-2023 08:15 til
        19-05-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   23-05-2023 10:15 til
        23-05-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   26-05-2023 08:15 til
        26-05-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science (MathBio)

time   30-05-2023 08:15 til
        30-05-2023 12:00

location   27.1-052 - lokale 2 (20)

Teacher   Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science - Hand-in of portfolio (MathBio)

time	12-06-2023 10:00 til 12-06-2023 10:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt

Scientific Computing and Data Science - Exam (MathBio)

time	15-06-2023 13:00 til 15-06-2023 14:15
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)

Scientific Computing and Data Science - Hand-in of portfolio (reexam) (MathBio)

time	30-06-2023 10:00 til 30-06-2023 10:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt

Scientific Computing and Data Science - Reexam (MathBio)

time	03-08-2023 08:15 til 03-08-2023 16:00
location	27.1-052 - lokale 2 (20)
Teacher	Thomas Schrøder (tbs@ruc.dk)