Statistical Physics with Scientific Programming

Title	Statistical Physics with Scientific Programming
Semester	E2022
Master programme in	Fysik / Mathematical Physical Modelling / 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	5
Responsible for the activity	Thomas Schrøder (tbs@ruc.dk)
Head of study	Kristine Niss (kniss@ruc.dk)
Teachers	
Study administration	INM Studieadministration (inm-studieadministration@ruc.dk)
Exam code(s)	U60192

ACADEMIC CONTENT

Overall objective	To give the student in-depth understanding of advanced thermodynamics and statistical physics, including: ● Free energies and phases ● Boltzmann statistics ● Systems of interacting particles To give the student experience in the interplay between analytical and numerical methods as applied to these subjects. To give the student exemplary knowledge and understanding of the strengths and limitations of analytical and numerical methods in the above contexts so that the student can recognize these when the methods are applied in other contexts
Detailed description of content	Statistical physics investigated via analytical and numerical methods, as well as simulations. Subjects include: ● Free energy and phases. ● Boltzmann statistics ● Systems of interacting particles. Numerical calculations and simulations are performed using Python, numpy and numba.
Course material and Reading list	Book: D. V. Schroeder, "Thermal Physics", International Edition, Addison Wesley Longman, ● Ch. 5: Free Energy and Chemical Thermodynamics ● Ch. 6: Boltzmann Statistics ● Ch. 8: Systems of interacting Particles Content of own mini-projects (including subjects that are left out, but ought to be included).
Overall plan and expected work effort	5 ECTS course ● Reading course material and problem solving at home: 35 hrs ● Discussion and problem solving in class: 15 hrs ● Working on mini-projects at home: 45 hrs ● Working on mini-projects in class: 30 hrs ● Exam preparation: 9 hrs ● Exam: 1 hours - **Total 135 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 0: Introduction to Scientific Programming in Python using numpy and numba - Theme 1: Boltzmann statistics. First mini-project: Boltzmann statistics of simple systems - Theme 2: Systems of interacting Particles. Second mini-project: Gas-liquid co-existence - Theme 3: Free energy and phases. Third mini-project: Extension of gas-liquid model

ASSESSMENT

Overall learning outcomes	After completing the course, the students will be able to - apply in-depth knowledge and understanding of free energies and Boltzmann statistics to new problems - understand and demonstrate in-depth knowledge of systems of interacting particles and analyse such systems - apply numerical and simulations methods to models in statistical physics. This includes the relevant programming, testing, and analysis of data.
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 portfolio 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 in the written part of the exam by their ability to:

- apply in-depth knowledge and understanding of free energies and Boltzmann statistics to models treated in mini-projects
- demonstrate understanding and in-depth knowledge of systems of interacting particles and ability to analyze such systems
- apply numerical and simulation methods to models in statistical physics. This includes the relevant programming, testing, and analysis of data.

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) : U60192

Course days:

Hold: 1

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	06-09-2022 13:15 til 06-09-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	08-09-2022 12:15 til 08-09-2022 16:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	13-09-2022 13:15 til 13-09-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	20-09-2022 13:15 til 20-09-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	22-09-2022 12:15 til 22-09-2022 16:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	27-09-2022 13:15 til 27-09-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	04-10-2022 13:15 til 04-10-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) – Room: Fysik B in building 27

time	06-10-2022 12:15 til 06-10-2022 16:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) – Room: Fysik B in building 27

time	11-10-2022 13:15 til 11-10-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) – Room: Fysik B in building 27

time	18-10-2022 13:15 til 18-10-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) – Room: Fysik B in building 27

time	20-10-2022 12:15 til 20-10-2022 16:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) – Room: Fysik B in building 27

time	01-11-2022 13:15 til 01-11-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	03-11-2022 12:15 til 03-11-2022 16:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	08-11-2022 13:15 til 08-11-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	15-11-2022 13:15 til 15-11-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	17-11-2022 12:15 til 17-11-2022 16:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming (PSM) - Room: Fysik B in building 27

time	22-11-2022 13:15 til 22-11-2022 15:00
Teacher	Thomas Schrøder (tbs@ruc.dk)

Statistical Physics with Scientific Programming - Hand-in of portfolio (PSM)

time	03-01-2023 10:00 til 03-01-2023 10:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt

Statistical Physics with Scientific Programming - Exam (PSM)

time	09-01-2023 08:15 til 09-01-2023 16:00
location	27.2-054 - lokale 3 (40)

Statistical Physics with Scientific Programming - Hand-in of portfolio (reexam) (PSM)

time	08-02-2023 10:00 til 08-02-2023 10:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt

Statistical Physics with Scientific Programming - Reexam (PSM)

time	15-02-2023 08:15 til 15-02-2023 16:00