Theory and Modelling in Natural Sciences

/ Teori och modellering inom naturvetenskap/

The research subject *Theory and modeling in natural sciences* covers the following subject areas:

Theoretical Physics/ Teoretisk fysik/SCB koder: 10304, 10302, 10399/

Computational Chemistry/ Beräkningskemi/SCB kod: 10407/

Theoretical Biology/Teoretisk biologi/SCB kod: 10611, 10699/

Bioinformatics/ Bioinformatik /SCB kod: 10203/

1 General description of the research subject

A unifying theme of the research subject *Theory and modeling in natural sciences* is theoretical research with a focus on theory, method development, modeling, simulations, and the processing and analysis of research data. These methodologies span many scientific disciplines represented by the subject areas of the doctoral education. The program is designed to develop doctoral students' analytical and quantitative skills in theoretical research, improve their ability to formulate and test scientific hypotheses, and provide experience with complex computer calculations and large-scale data analysis.

Research based on theory and modeling uses models to describe complex real-world systems in ways that are practically manageable without losing necessary flexibility. These models are built on fundamental equations, and their solutions provide insights into the systems' properties. The solution of these equations often requires developing new methods that are implemented in software and simulated using computers. The outcome can then be analyzed to determine if the model is useful for extracting new and useful knowledge, or if it needs to be revised. Simulation data produced this way is often collected and made available in research databases and used in, for example, data-driven analysis with techniques such as informatics and AI. The approach is universally applicable in theoretical research and development activities, and our ambition is to ensure that the doctoral education provides a solid foundation for future work in R&D both in the academic and industrial sectors.

2 Eligibility requirements and selection

The basic eligibility requirements as well as the general principles for selection are specified in the faculty's *Study Handbook for PhD Studies*.

2.1 Specific eligibility requirements

Entitled to be admitted to PhD Studies in the research subject of *Theory and modeling in natural sciences* is anyone who has completed the course requirements of at least 60 ECTS at master's level related to the respective subject area. These 60 ECTS must include an independent work (degree thesis) with a scope of at least 30 ECTS in an area relevant to the subject area.

3 Degree

PhD studies in *Theory and modeling in natural sciences* lead to a Degree of Doctor or a Degree of Licentiate. The latter degree can also serve as a stage in the PhD studies. The Degree of Licentiate comprises 120 ECTS, of which courses correspond to studies of 30 higher education credits for the subject areas of theoretical biology, computational chemistry and bioinformatics, as well as 45 higher education credits for theoretical physics. Of these, at least 20 ECTS for the subject areas of theoretical biology, computational chemistry and bioinformatics, as well as at least 30 higher education credits for theoretical physics must be at PhD level. The thesis work corresponds to studies of 90 ECTS for theoretical biology, computational chemistry and bioinformatics and 75 ECTS for theoretical physics. The doctoral degree comprises 240 ECTS, of which courses correspond to studies of 60 ECTS for theoretical biology, computational chemistry and bioinformatics, as well as 90 ECTS for theoretical physics. Of these, at least 40 ECTS for the subject areas of theoretical biology, computational chemistry and bioinformatics, as well as at least 60 ECTS for theoretical physics must be at PhD level. The thesis work corresponds to studies of 180 ECTS for theoretical biology, computational chemistry and bioinformatics and 150 ECTS for theoretical physics.

4 Goals and implementation of the PhD studies

The general outcomes and objectives of PhD studies are specified in the introduction to the faculty's *Study Handbook for PhD Studies*, as well as in the Higher Education Ordinance (reprinted in the *Study Handbook*'s appendix A).

The PhD studies in the research subject of Theory and Modeling in Natural Sciences provide the PhD student with the prerequisites to meet all the degree outcomes. The PhD studies consist of research and thesis work, courses, participation in seminars, involvement in national and international conferences, and collaboration with industry. The PhD studies provide the PhD student with broad and deep knowledge and understanding in Theory and Modeling through a selection of the following components: the PhD student takes basic and comprehensive courses as well as courses in their research area within their research focus, participates in the teaching of undergraduate courses, works with research projects, participates in interdisciplinary doctoral schools, and prepares and presents their research at national and international conferences.

The PhD student acquires deep knowledge and understanding of the research subject by actively participating in relevant courses in mathematical modeling, statistics, programming, visualization, database management, informatics, data-driven analysis, and the development and use of AI models.

The PhD student develops familiarity with scientific methodology by applying the methodology of the research field in their own research and by completing a mandatory course in research methodology.

PhD students in the research subject Theory and Modeling in Natural Sciences acquire skills and abilities by:

- Reviewing and modeling various systems relevant to their research focus.
- Independently planning and conducting their research.
- Demonstrating the ability to contribute to the development of knowledge in theory and modeling through their own research.
- Participating in the research group's meetings, seminars, guest lectures, and similar activities. This includes presenting achieved research results and plans for the continued thesis work at least once a year.
- Preparing and presenting a half-time seminar or licentiate seminar before the licentiate exam or after completing approximately 60% of the doctoral coursework requirements.
- Participating in conferences and presenting their own research. This develops the ability to present their work to colleagues and withstand critical scrutiny.
- Taking courses in areas such as presentation techniques, leadership, management, entrepreneurship, media training, methodology/ethics, and/or pedagogy.
- Participating in science popularization activities.

The above provides the PhD student with good prerequisites to contribute to societal development both in research and education, as well as in other qualified professional contexts, and to support others' learning within the chosen direction of the field of Theory and Modeling.

The PhD student develops critical thinking and attitudes within the research subject Theory and Modeling in Natural Sciences, for example, by:

- Creating intellectual independence and scientific integrity to conduct their own research within Theory and Modeling in Natural Sciences.
- Completing a mandatory course in research ethics.
- Participating in the research group's seminar activities or group meetings.
- Engaging in internal and/or external research collaborations.
- Training in both giving constructive feedback on others' research and responding to constructive feedback on their own research.

PhD students in the research subject Theory and Modeling in Natural Sciences demonstrate intellectual independence by independently driving research projects and presenting the results in various internal and external contexts, as well as writing a thesis. The PhD student develops their oral and written communication and critical thinking by regularly (at least once per year) presenting achieved results and plans for the continued thesis work in a seminar series within the research environment.

The studies provide the PhD student with a deeper understanding of how science can contribute to sustainable societal development. This is achieved through mandatory learning activities as well as through participation in ongoing discussions in, for example, research seminars and through reflection on the sustainability aspects of their own research work.

4.1 Thesis

The overall rules regarding the format, submission and grading of a thesis can be found in the faculty's *Study Handbook for PhD Studies*.

The PhD student demonstrates her/his ability to make a significant contribution to the development of knowledge through their own research by writing a doctoral thesis or a licentiate thesis, whose scientific quality must be approved by an examination committee (for the doctoral thesis) or an examiner (for the licentiate thesis).

4.1.1 Doctoral thesis

A doctoral thesis can be a monograph or a compilation thesis. A compilation thesis for a PhD degree in Theory and Modeling in Natural Sciences consists of a summarizing text and a number of attached scientific articles that have been accepted for publication in established scientific journals, conferences, or books, or meet reasonable requirements to be accepted for such publication. The articles must constitute a significant and innovative contribution to the research field that meets the standards of quality, originality, and scientific impact that have been established for a PhD degree within the specific research area. During the public defence, it is the task of the assessment committee to ensure that the thesis meets these requirements. A monograph must maintain an equivalent high scientific standard.

4.1.2 Licentiate thesis

A licentiate thesis can be a monograph or a compilation thesis. A compilation thesis for a licentiate degree in Theory and Modeling in Natural Sciences typically consists of a summarizing text and one or more articles, similar to a doctoral thesis, where at least one article has been accepted for publication in an established scientific journal, conference, or book, and the remaining articles are assessed to meet reasonable standards for acceptance for publication. A monograph should maintain an equivalent high scientific standard.

4.2 Individual study plan

An individual study plan will be formulated for each PhD student. The detailed planning of courses and other components will be conducted in consultation with the supervisor and documented in the individual study plan (see *Study Handbook for PhD Studies*, section 5.3). The study plan should be established within one month after admission to PhD studies, and it should be revised at least once a year.

4.3 Supervision

The general regulations for supervision can be found in the *Study Handbook for PhD Studies*, section 4, and in the faculty's policy for supervision of PhD studies.

A main supervisor is appointed for each PhD student. In addition, one or more co-supervisors should be appointed. The role of the supervisors is to guide the student throughout her/his studies, including advising on course selection and choosing research tasks. The student and supervisors are expected to have regular meetings to discuss and consult on the progress of the research work.

4.4 Courses

4.4.1 Faculty course requirements

Scientific theory, methodology, ethics, gender equality and sustainability
All PhD students admitted should complete mandatory courses as decided by the faculty in scientific theory, methodology, ethics, gender equality and sustainability, or be deemed to have equivalent competencies, in order to receive a degree.

Pedagogic studies
All PhD students who teach should complete a basic course in pedagogy. At least 3 ECTS from this course should be included in the PhD studies, and any remaining credits should be counted as departmental duties (see *Study Handbook for PhD Studies*, section 5.5).

4.4.2 Subject related courses

PhD courses in mathematical modeling, statistics, programming (especially for high-performance computing), visualization, database management, informatics, data-driven analysis, and the development and use of AI models are considered highly relevant for the doctoral program subject. There is a general recommendation to prioritize courses in these areas. PhD students are also encouraged to participate in national and international intensive courses (so-called summer schools) within their respective research fields.

4.4.3 Other subject related mandatory components

The PhD studies include the following mandatory components regarding the presentation of the student's own research:

- Studies for a licentiate degree must include participation and presentation of the student's own research at least once at a national or international scientific meeting.

- Studies for a PhD degree must include participation and presentation of the student's own research at least twice at scientific conferences, with at least one presentation at a major international scientific meeting and at least one presented orally at a national or international scientific meeting.

4.4.4 Accreditation

Accreditation of course credits is regulated by the *Study Handbook for PhD studies*, section 5.6.

5 Subject areas

5.1 Theoretical physics

PhD studies in theoretical physics build on the fundamental laws of physics to achieve a microscopic understanding of physical processes and properties of materials. The primary areas include condensed matter theory, nanoscience, quantum physics, electromagnetic modeling, and nonlinear physics. A key theme is the development of new and improved materials for various applications, which is enabled by an understanding of the relationship between structure and properties. The work is closely integrated with experimental work both at the Department of Physics, Chemistry, and Biology (IFM) and beyond. This interplay between theory and experiment is a cornerstone and driving force for the research in theoretical physics. An important objective of education in theoretical physics is to provide PhD students with in-depth knowledge and understanding of the theoretical fundamentals of quantum mechanics, statistical mechanics, and solid-state physics. Additionally, the program provides the knowledge and skills to carry out numerical simulations on high-performance computers.

5.1.1 Mandatory courses

For a PhD degree, the PhD course *Fundamental Principles of Theoretical Physics* (2 ECTS credits) is mandatory. For a licentiate degree, approval is required for a subset of the modules in this course, totaling at least 1 ECTS credit.

5.1.2 Area-specific course requirements

Specific core subjects within theoretical physics include quantum mechanics, statistical and thermal physics, solid-state physics, quantum information, electrodynamics, optics, materials science (including semiconductor physics, surface physics, nanophysics, material defects), density functional theory, group theory, elementary particle physics, chaos and nonlinear systems, plasma physics, and related applied subjects. This may also include courses related to the management of large-scale research data from theoretical simulations, including databases, AI methods (e.g., machine learning), semantic data description, and large-scale data analysis for PhD students with research projects connected to these subjects.

For a licentiate degree, at least 25 ECTS credits are required in core subject courses, and for a PhD degree, at least 45 ECTS credits are required in core subject courses.

5.2 Computational chemistry

PhD studies in computational chemistry address a range of different questions in chemistry and biology, which are explored using quantum chemical computational methods and methods of statistical thermodynamics. These questions typically originate from chemical and biological problems concerning the function, reactivity, and properties of molecules. Current research projects aim, among others, to establish photochemical reaction mechanisms, design molecular motors and switches for nanotechnological applications, and explore and develop surface chemical processes. An important goal of the doctoral studies in computational chemistry is to provide students with the skills to model the function, reactivity, and properties of molecules, to formulate and critically evaluate models in computational chemistry, to link theoretical research results with experimental studies, as well as to provide students with advanced subject knowledge in computational chemistry and the skills to conduct numerical simulations on high-performance computers.

5.2.1 Area-specific course requirements

Specific core subjects within computational chemistry include quantum mechanics, statistical and thermal physics, quantum chemistry, density functional theory, group theory and molecular symmetry, response theory, organic chemistry, surface chemistry, photochemistry, solid-state physics, and scientific programming.

For a licentiate degree, at least 20 ECTS credits are required in core subject courses, and for a PhD degree, at least 40 ECTS credits are required in core subject courses. For both the licentiate and PhD degrees, at least 6 ECTS credits must be earned in both quantum mechanics and statistical and thermal physics.

5.3 Theoretical biology

PhD studies in theoretical biology focus on the development and use of mathematical and statistical models, as well as the analysis of large data sets, to address questions in ecology and environmental science. A main area is the analysis of structure, dynamics, and functionality in complex ecological networks. Other key areas include statistical methods for modeling disease transmission in livestock and wildlife monitoring. The research emphasizes analysis and method development, with questions arising from biological processes, and analyses and methods based on mathematical or statistical models. Current research topics include ecosystem vulnerability to different types of disturbances, conservation of biological diversity in dynamic landscapes, pest control, the spread of infectious diseases, and efficient nutrient management in plant production. An important goal of doctoral education in theoretical biology is to provide students with skills to perform vulnerability analyses and risk assessments in biological systems, advanced subject knowledge in theoretical biology, and proficiency in mathematical modeling, statistics, and programming.

5.3.1 Mandatory courses

The mandatory course is: *Seminar Activities in Biology*, 10 ECTS credits.

5.3.2 Area-specific course requirements

Specific core subjects within theoretical biology include theoretical ecology, epidemiology, evolution, mathematical analysis, statistics, programming, and database management.

For a licentiate degree, at least 20 ECTS credits are required in core subject courses, and for a PhD degree, at least 40 ECTS credits are required in core subject courses.

5.4 Bioinformatik

PhD studies in bioinformatics focus on methods for interpreting and understanding the information in the genome, DNA, and mapping the functions of proteins. The research is aimed at developing methods for data management, predictions, and linking experiments to modeling. Additionally, existing methods are used to solve biologically and medically relevant problems, often in collaboration with other research groups. Examples of research areas include the use of molecular modeling to study dynamic processes, method development for predicting protein structure and function, predictions of protein-protein interactions, analysis of data from large-scale sequencing, and the construction and analysis of gene and protein networks.

5.4.1 Area-specific course requirements

The subject area of bioinformatics also has a requirement that at least 40 ECTS credits for a PhD degree and at least 20 ECTS credits for a licentiate degree must be in subjects directly relevant to the field: biophysics, molecular physics, biochemistry, molecular biology, genetics, protein chemistry, structural biology, structure and dynamics of complex biological systems, visualization, bioinformatics methods, programming and computer science, machine learning methods, statistics and database management, as well as courses in handling large-scale data sets.

6 Other information

6.1 Transitional provisions

Changes to the general study syllabus do not apply to those who have already been admitted to PhD studies in the research area. A change to the new general study syllabus may however be approved if both the main supervisor and the PhD student agree. In such a case, this should be documented in the individual study plan.

7 Commencement

1. The General Study Syllabus comes into force on 1st of July 2024.