

Theory and Modelling in Natural Sciences

/Teori och modellering inom naturvetenskap/

The governing rules common for all PhD Studies at Linköping University's Institute of Technology can be found in the faculty's *Study Handbook for PhD Studies*. Some overall rules can also be found in Linköping University's local rules and regulations as well as in the Higher Education Act and the Higher Education Ordinance.

The research area Theory and Modelling in Natural Sciences includes four specialisations:

- **Theoretical Physics**/ Teoretisk fysik/ SCB codes: 10304, 10302, 10399/
- **Computational Chemistry**/ Beräkningskemi/ SCB code: 10407/
- **Theoretical Biology**/ Teoretisk biologi/ SCB codes: 10611, 10699/
- **Bioinformatics**/ Bioinformatik/ SCB code: 10203/

General description of the research area

The research conducted within the research area of Theory and Modelling in Natural Sciences has a broad scientific profile and shares a common core of mathematical modelling, numerical methods and computer simulations.

The research can essentially be divided into four main parts, namely, modelling, method development, numerical simulation and analysis. A model is developed to describe the complex reality in a practically manageable way, without losing the necessary flexibility. The model will consist of a number of basic equations whose solutions describe the system properties. Solving these equations often requires development of new methods that can be implemented in software and simulated on computers. Analysis of the results shows whether new and useful knowledge can be extracted from the model, or if the model needs to be modified. This approach is generally applicable in theoretical research and development, and it is our ambition that the PhD Studies should provide a solid foundation for continued work within research and development in academia as well as in industry.

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*. Details regarding how the selection is made are specified in the respective announcements for the positions.

Specific eligibility requirements

Admission to PhD Studies in the research area of Theory and Modelling in Natural Sciences requires completion of courses of at least 60 ECTS at the master level in these areas: theoretical physics, theoretical biology, computational chemistry or bioinformatics. The candidate should have carried out a substantial project (degree project) of at least 30 ECTS in a field relevant to the subject of PhD studies: theoretical physics, theoretical biology, computational chemistry or bioinformatics.

- Moreover, the specific eligibility requirements for Theoretical Physics include passing undergraduate courses in subjects of quantum mechanics, thermodynamics and statistical physics, classical electrodynamics and solid state physics. Exemption from specific eligibility requirements may be made in exceptional circumstances. Such decisions will be made in

consultation with the main supervisor and the Director of PhD studies at the relevant department.

Degree

PhD studies in Theory and Modelling 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 30 ECTS in the specialisations Theoretical Biology, Computational Chemistry and Bioinformatics, and to 45 ECTS in the specialisation Theoretical Physics. The licentiate thesis corresponds to 90 ECTS for Theoretical Biology, Computational Chemistry and Bioinformatics, and to 75 ECTS for Theoretical Physics.

The Degree of Doctor comprises 240 ECTS, of which courses correspond to 60 ECTS for Theoretical Biology, Computational Chemistry and Bioinformatics, and to 90 ECTS for Theoretical Physics. The doctoral thesis corresponds to 180 ECTS for Theoretical Biology, Computational Chemistry and Bioinformatics, and to 150 ECTS for Theoretical Physics.

Goals and implementation of the PhD studies

The general goals 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).

PhD studies in the research area Theory and Modelling in Natural Sciences will equip the PhD student with the knowledge and skills to fulfill all the degree outcomes. The PhD studies will endow the PhD student with a broad knowledge and understanding of his/her area of research.

The PhD studies will give the PhD student broad and deep knowledge and understanding of the research area through a selection of the following activities: the PhD student will take basic and wide-ranging courses as well as in-depth courses within his/her area of research in his/her specialisation, help to teach undergraduate courses, work with research projects, participate in the multidisciplinary graduate schools' work, and prepare and deliver presentations about his/her research at national and international conferences.

More specifically, the PhD student will acquire deep knowledge and understanding of the research area by attending courses within the core of the research area. Examples of general core subject courses in Theory and Modelling in Natural Sciences are courses in mathematical modelling, statistics, scientific computing, different programming languages, visualisation and maintaining of databases. Examples of specific core subject courses in

- The specialisation Theoretical Physics are courses in solid state physics, statistical and thermal physics, and quantum mechanics
- The specialisation Computational Chemistry are courses in in computational/theoretical chemistry and statistical thermodynamics
- The specialisation Theoretical Biology are courses in theoretical ecology, evolution and mathematical modelling of biological systems
- The specialisation Bioinformatics are courses in in biophysics, molecular physics, biochemistry, molecular biology, genetics, proteins chemistry, structure and dynamics of complex biological systems, bioinformatics methods and machine learning methods.

The PhD student will develop familiarity with scientific methodology through his/her own research and by attending a mandatory course in research methodology.

PhD students in the research area of Theory and Modelling in Natural Sciences will acquire skills and competencies:

- By examining and modelling different systems relevant to the area of specialisation.
- By independently planning and carrying out theoretical research.
- By demonstrating the ability to contribute to the development of knowledge in Theory and Modelling through own research.
- By participating in the research group's meetings or seminars. This includes reporting the attained results and presenting plans for continued thesis work at least once a year.
- By participating in conferences and presenting at such fora research results. This will train the student's ability to present his/her work to colleagues and to subject him-/herself to critical review.
- By participating in so-called non-core subject courses such as presentation techniques, leadership, management, entrepreneurship, media training, methodology/ethics and/or pedagogy.
- By participating in activities to popularise science.

The above-mentioned activities will equip the PhD student with the skills and knowledge to contribute to social development and encourage learning by others both in the world of research and education and in other qualified professional contexts in the field of Theory and Modelling.

PhD students in the research area of Theory and Modelling in Natural Sciences will develop judgement and scientific approach by, for example:

- Cultivating intellectual independence and disciplinary rectitude in conducting own research in Theory and Modelling in Natural Sciences
- Attending a mandatory course in research ethics
- Participating in the research group's seminars or group meetings
- Participating in internal and/or external research collaborations
- Practising the ability to critically and constructively review others' results and articles, and at the same time learning how to receive and respond to criticism.

PhD students in the research area of Theory and Modelling in Natural Sciences will demonstrate their intellectual autonomy by independently conducting a research project and presenting attained results in various internal and external settings, as well as by writing a thesis. PhD students will develop their oral and written communication skills as well as their critical thinking by regularly (at least once a year) reporting on attained results and plans for continued thesis work in a seminar series.

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*.

- a) Doctoral thesis

The extent of the scientific research should correspond to at least three years of full-time research work (2,5 years for the specialisation Theoretical Physics). The research results are submitted in a doctoral thesis, which can be presented either as a continuous piece of work or as a compilation of scientific essays.

The thesis should be of such level of quality that it, in its entirety, can be judged to meet reasonable requirements to be accepted for publication in scientific journals of good quality. In a compilation thesis, the greater part of the included works should be published or accepted for publication

Licentiate thesis

The extent of the thesis work should correspond to at least 1,5 years of full-time work (1,25 years for the specialisation Theoretical Physics). The thesis can consist of one or several scientific essays and/or an investigative report conducted on scientific grounds.

Both types of theses can be done as part of teamwork, but the student's contribution should consist of independent work and be specifically accounted for in the thesis' introduction.

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.

Supervision

General rules governing supervision of PhD studies can be found in Chapter 4 of the *Study Handbook for PhD Studies* and in the *Policy for the Supervision of PhD Studies*.

At the beginning of PhD studies, a main supervisor will be appointed for each PhD student. Moreover, one or more co-supervisors will be appointed. The supervisors' roll is to guide the student during the period of study regarding, among other things, course selection and selection of research projects. The student and the supervisors should meet regularly to discuss and consult on the progress of the research work.

Courses

Courses in the research area of Theory and Modelling in Natural Sciences are divided into courses within general core subjects, specific core subjects and non-core subjects.

Faculty course requirements

Scientific theory, methodology and ethics

All PhD students admitted as of 1 January 2010 should complete mandatory courses as decided by the faculty in methodology and ethics, 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).

General core subjects

General core subjects are mathematical and physical modelling, statistics, programming, scientific computing, large scale databases, machine learning.

Other mandatory components

PhD studies include mandatory components involving the presentation of the PhD student's own research. These components may count toward the degree as PhD courses and give 2 ECTS for a Degree of Licentiate and 5 ECTS in total for a Degree of Doctor. The mandatory components are as follows:

- Studies toward a Degree of Licentiate should include participation and presentation of own research at at least one national or international scientific meeting/conference. This may count toward the degree as a PhD course and give 2 ECTS.
- Studies toward a Degree of Doctor should include participation and presentation of own research at at least one large international scientific meeting/conference as well as oral presentation of own research at at least one national or international scientific meeting/conference. These activities may count toward the degree as a PhD course and give 3 ECTS.

Recommended courses

There is a general recommendation to prioritise core subject courses. PhD students are encouraged to participate in national and international intensive courses (so-called summer schools) within their respective specialisations. A course in scientific computing on high-performance computers is recommended.

Courses within non-core subjects

Besides courses within core subjects, the PhD student can also select courses in non-core fields (e.g. presentation techniques, leadership, intellectual property law, project management, entrepreneurship, media training, scientific publishing, etc.).

Accreditation

Master courses that are equivalent to at most 15 ECTS for a Degree of Licentiate and 30 ECTS for a Degree of Doctor, that do not form part of the basic or specific eligibility requirements for the specialisation, and that are relevant to the PhD studies, may be counted toward the degree. The PhD student should submit an application for accreditation using the appropriate form; the application is to be approved or rejected by the main supervisor, and a positive decision on accreditation can be made by the Director of PhD Studies at the relevant department. A decision to reject an application for accreditation may not be made by the Director of PhD Studies at the department, rather, such a decision can only be made by the faculty's Board of PhD Studies.

Specialisations

Theoretical Physics

Research and PhD studies in theoretical physics are based on the fundamental laws of physics, from which understanding at microscopic level of physical processes and material properties are sought. The research is primarily focused on condensed matter theory, nanoscience, quantum physics, electromagnetic modelling and non-linear physics; one example of a main research theme is how understanding the connection between structure and properties of materials can contribute to the development of new and improved materials in a number of application areas. The work is closely related to experimental activities at the department IFM and outside, and this interplay between theory and experiment is the core and driving force for the research in theoretical physics. An important aim of the PhD Studies in theoretical physics is to give PhD students a profound knowledge and understanding of the theoretically basic subjects quantum mechanics, statistical mechanics and solid state physics, as well as providing knowledge and skills to perform numerical simulations on high performance computers.

Specialisation-specific course requirements

Specific core subjects for the specialisation Theoretical Physics are analytical mechanics, quantum mechanics, quantum information, thermodynamics and statistical mechanics, electrodynamics, fluid mechanics, optics, solid state physics, materials science (including semiconductor physics, surface physics, nanophysics, materials defects), density functional theory, theory of relativity, differential geometry and topology, group theory, cosmology and astrophysics, elementary particle physics, chaos and non-linear systems, nuclear physics, plasma physics, string theory, as well as associated applied subjects.

Courses are divided into advanced undergraduate level and PhD level.

Distribution of course credits

For a Degree of Licentiate, at least 25 ECTS are required within core subject courses (of which 15 ECTS in Theoretical Physics). For a Degree of Doctor, at least 45 ECTS are required within core subject courses (of which 30 ECTS in Theoretical Physics).

Mandatory courses

Mandatory courses are: Quantum mechanics (6 ECTS), Statistical and Thermal physics (6 ECTS), Solid state physics (6 ECTS). For a Degree of Licentiate, only two of the three core subject courses are mandatory.

Computational Chemistry

Research and PhD studies in computational chemistry are concerned with a wide variety of problems in chemistry and biology, which are investigated using computational techniques ranging from quantum chemical methods to methods rooted in statistical thermodynamics. The problems of interest are typically related to the function, reactivity and properties of molecular systems in different chemical and biological contexts. Current research projects focus on providing a better understanding of photochemical reaction mechanisms, designing and developing improved molecular machines for applications in nanotechnology, and facilitating efficient procedures for chemical synthesis on surfaces. Important goals of the education are to provide the student with skills in modelling the

function, reactivity and properties of molecular systems, experience in formulating and critically evaluating models in computational chemistry, practice in relating computational research data to experimental studies, proficiency in executing numerical simulations using high-performance computing resources, as well as in-depth knowledge of the field.

Specialisation-specific course requirements

Specific core subjects for the specialisation Computational Chemistry are computational chemistry, quantum chemistry, response theory, surface chemistry, photochemistry, statistical thermodynamics, density functional theory, scientific programming, quantum mechanics and solid state physics.

Distribution of course credits

For a Degree of Licentiate, at least 20 ECTS are required within core subject courses (of which 10 ECTS in Computational Chemistry/Theoretical Chemistry). For a Degree of Doctor, at least 40 ECTS are required within core subject courses (of which 20 ECTS in Computational Chemistry/Theoretical Chemistry).

Mandatory courses

Mandatory courses are: Quantum mechanics (6 ECTS).

Theoretical Biology

Research and PhD studies in theoretical biology deal mainly with the structure and dynamics of complex ecological networks. Research is focused on analysis and method development. Research topics are based on biological processes. Analysis and methods are based on mathematical or statistical models. Examples of current studies are ecosystem vulnerability to different types of disturbances, biodiversity conservation in dynamic landscapes, control of pests, spread of infectious diseases, and efficient nutrient management in plant production. An important goal of education in theoretical biology is to give students the skills to carry out vulnerability analysis and risk assessment in biological systems, in-depth knowledge of the subjects in theoretical biology, as well as providing knowledge and skills in mathematical modelling, statistics and programming

Specialisation-specific course requirements

Specific core subjects for the specialisation Theoretical Biology are theoretical ecology, epidemiology, evolution, mathematical analysis, programming, database processing.

Distribution of course credits

For a Degree of Licentiate, at least 20 ECTS are required within core subject courses. For a Degree of Doctor, at least 40 ECTS are required within core subject courses.

Mandatory courses

Mandatory courses are: PhD student seminar in the subject of biology.

Bioinformatics

Research and PhD studies in bioinformatics deal with methods for understanding biological

data, such as genome, DNA, RNA. The research is focused on the development of methods to solve biologically and medically relevant problems, often in collaboration with other research groups. Examples of research areas include: the use of molecular modelling to study dynamic processes and methods for the prediction of the structure and function of proteins, prediction of protein-protein interactions, analysis of data from large-scale sequencing, as well as for the design and analysis of gene and protein networks

Specialisation-specific course requirements

Specific core subjects for the specialisation Bioinformatics are biophysics, molecular physics, biochemistry, molecular biology, genetics, protein chemistry, structure and dynamics in complex biological systems, visualisation, bioinformatics methods, programming courses, machine learning methods, statistics, and databases.

Distribution of course credits

For a Degree of Licentiate, at least 20 ECTS are required within core subject courses. For a Degree of Doctor, at least 40 ECTS are required within core subject courses.

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.