LUND UNIVERSITY

FACULTY OF SCIENCE

Programme sheet

Master Programme in Applied Computational Science, Chemistry, 120 credits

September 2023 – June 2025

Computations are becoming more and more important in research and industry. To make predictions, analysis or to replace experiments, we make use of numerical simulations and machine learning on large computers. We generate and store large amounts of data and use data science to search for patterns, connections, and trends.

The Master Programme in Applied Computational Science with specialisation in Chemistry will give you detailed knowledge about the underlying methods with respect to chemistry. You will learn how to study complex processes in natural sciences, and how Computational Science can contribute to knowledge evolution in society. A few of many examples are studies in, and research on, environment and climate change, climate adaptation, biodiversity and ecosystem services, nature conservation and chemical risks. The programme will prepare you for a professional career in academia as well as in business and industry. Applied computational science can be divided into several components: mathematics, modelling, statistics, and programming. The borders are not sharp, as concepts and methods often combine these components. The programme will prepare you for a professional career in academia as well as in business and industry.

Programme overview

This interdisciplinary education will give you in-depth knowledge in the field of computational science, but you also study advanced courses

based on your subject knowledge in chemistry from your bachelor's degree. In addition to knowledge of theory of computational science, there will be an emphasis on obtaining knowledge about the practical tools that are used by professionals in the field and you will amongst several things train your skills in programming. You will get generic knowledge and skills of importance for computationally intensive jobs such as problem formulation, information search, data processing, scientific writing, and presentation techniques.

The programme has five separate specialisations: Environmental Science, Biology, Geology, Physical Geography and Chemistry. You will study several courses together with students from another specialisation than your own and there are possibilities to do common projects and thesis work. During your studies, an interdisciplinary perspective is emphasized and you will even study together with students from mathematics and physics.

The education has a strong connection to research. You will meet and be taught by active and internationally well recognised researchers, and you will be in contact with several research groups. You will at the same time be prepared for a career in business and industry.

Programme structure

With a specialisation in Chemistry, you will first study the mandatory course Molecular Driving Forces and Chemical Bonding, KEMM30. This course includes statistical data analyses, using Python programming. Also included are computationally relevant parts, such as Statistical Thermodynamics, Quantum Mechanics, Intermolecular Interactions, and Spectroscopy. The next course within the programme is Mathematics for Scientist 2. During the first half of the second semester, we recommend master level courses in Statistical Mechanics and Molecular Simulation (KEMM48) as well as Molecular Quantum Mechanics (KEMM58). During the final half of the spring semester, the programme provides courses in Biostatistics, and Computational Programming using Python. The second year includes two compulsory courses: Computational Science, and Reproducible Data Science and Statistical Learning. We also recommend applied master courses withing the field of Chemistry. The final semester is devoted to an exam project.

Compulsory courses 60 credits

KEMM30	Molecular Driving Forces and Chemical Bonding, 15 credits
MATA04	Mathematics for Scientists 2, 15 credits
MASB11	Biostatistics - Basic Course 7.5 credits
NUMA01	Computational Programming with Python, 7.5 credits
BERN01	Modelling in Computational Science, 7.5 hp
BERN02	Reproducible Data Science and Statistical Learning, 7.5 credits

Elective courses, at least 30 credits

KEMM48	Statistical Thermodynamics and Molecular Simulation, 7.5 credits
KEMM58	Molecular Quantum Mechanics, 7.5 credits
KEMM77	Advanced Surface and Colloid Chemistry, 15 credits
MNXB01	Introduction to Programming and Computing for Scientists, 7.5 credits
FYSN17	Quantum Mechanics, 7.5 credits
FYST13	Chaos for Science and Technology, 7.5 credits
FYTN14	Introduction to Artificial Neural Networks and Deep Learning, 7.5 credits
BERN03	Introduction to Modelling of Climate Systems, 7.5 credits
STAE02	Bayesian Methods, 7.5 credits
KEMM67	Scattering Methods, 7.5 credits
KEMM57	Magnetic Resonance - Spectroscopy and Imaging, 7.5 credits
KEMM29	Molecular Spectroscopy - Methods and Applications, 15 credits
FYST19	Physics and Chemistry of Surfaces, 7.5 credits

Degree project 30 credits

BERMXX	Degree project Master of Science, 30 credits

Table 1 Course of study, example.

Year 1	Autumn 1	Autumn 2	Spring 1	Spring 2
	KEMM30 Molecular Driving Forces and Chemical Bonding, 15 credits	**MATA04** Mathematics for Scientists 2, 15 credits	KEMM48 Statistical Thermodynamics and Molecular Simulation, 7.5 credits	**MASB11** Biostatistics, 7.5 credits
			KEMM58 Molecular Quantum Mechanics, 7.5 credits	**NUMA01** Computational Programming with Python, 7.5 credits
Year 2	**Autumn 1**	**Autumn 2**	**Spring 1**	**Spring 2**
	BERN01 Modelling in Computational Science, 7.5 credits	KEMM77 Advanced Surface and Colloid Chemistry, 15 credits	**Degree project Master of Science, 30 credits**	
	BERN02 Reproducible Data Science and Statistical Learning, 7.5 credits			

Career opportunities

After graduation, there are several different career paths depending on which subject profile you have chosen. The Master's programme gives you a solid ground for postgraduate education in natural sciences. You can also choose a career path outside academia and then find attractive jobs in areas where there is a need to solve computational problems both in industry and in public administration and other organisations.

Requirements and selection

Entry requirements

Bachelor´s degree of at least 180 credits, including 90 credits in science of which 15 credits should be in mathematics and 45 credits should be in chemistry*.

Proficiency in English equivalent to English 6/B from Swedish upper-secondary school.

or

Bachelor´s degree of at least 180 credits, including 90 credits in science of which 15 credits should be in mathematics and 75 credits should be in physics.

Proficiency in English equivalent to English 6/B from Swedish upper-secondary school.

**We strongly recommend that this should include 15 credits in physical chemistry.*

Selection criteria

Seats are allocated according to: Previous college/university studies (HPAV): 100 %.

Degree

Master of Science
Major: Applied Computational Science with specialisation in Chemistry
Naturvetenskaplig masterexamen
Huvudområde: Tillämpad beräkningsvetenskap med fördjupning i kemi

Application

Apply online using Universityadmissions.se
Application period: 17 October 2022 - 16 January 2023
Language of instruction: English

Contact

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