

Computational Science: Chemistry

Department of Chemistry, University of Oslo

Planned start: Fall 2018

Why Chemistry

One hundred years after the quantum mechanical revolution, chemistry has reached the level of a mature discipline, where the fundamental equations describing the interactions at the level of chemical bonding and intermolecular forces are in principle known. The grand challenge that we face today is in predicting and controlling with high accuracy the behaviour of chemical systems in the presence of complex interactions (heterogeneous phases, system not in thermodynamic equilibrium, interactions with strong electromagnetic fields, etc).

This is where computational modeling enters in the game – by taking this study direction, you will learn to develop and apply a variety of tools that allow you to describe chemical processes at different resolution scales: from solving very accurate quantum mechanical and electronic structure problems, through modeling chemical reactions in the gas phase as well as in solution, to modeling soft-matter and biological systems like proteins, DNA, and so on. Both software development and the constant growth of massive parallel architectures allow us to overcome the heavy computational costs in simulations of molecular systems. Graphical user interfaces are also important tools used today in modeling chemistry

In addition to the general skills acquired in the Master in Computational Science, here we note that computer modeling is today a standard tool used in several chemistry labs both in research and industry — for example, drug development research and development units use computer modeling to optimize leads prior to their synthesis, which will make the profile of the graduate students very appealing in the job market.

Structure and courses

The table here is an example of a suggested path for a Master of Science project, with course work the first year and thesis work the last year.

	10 ECTS	10 ECTS	10 ECTS
4th semester	Master thesis	Master Thesis	Master Thesis
3rd semester	Master thesis	Master Thesis	Master Thesis
2nd semester	Master courses	Master courses	Master courses
1st semester	Master courses	Master courses	Master courses

This program is very flexible in its structure and students may opt for starting with their thesis work from the first semester and scatter the respective course load across all four semesters. Depending on interests and specializations, there are many courses on computational science which can make up the required curriculum of course work. Furthermore, courses may be broken up in smaller modules, avoiding thereby the limitation of 10 ECTS per course only. Some of these courses are listed below.

Courses. Depending on specialization, the following courses that can be included as part of the compulsory 60 ECTS needed for a Master of Science degree are [described here](#).

Students have to choose among two of the following courses

1. CS-MATH1 (data analysis and machine learning)
2. CS-MATH2 (mathematical modeling)
3. CS-INF1 (High performance computing)

The following courses are recommended for students in this study direction:

1. FYS3150/4150 Computational Physics I
2. FYS4411/9411 Computational Physics II (Computational quantum mechanics with an emphasis on Quantum Monte Carlo, Hartree-Fock, Coupled Cluster, FCI)
3. FYS4460/9460 Computational Physics III (Computational statistical mechanics with an emphasis on Molecular dynamics, percolation and critical phenomena)
4. **CS-PHYS6:** Computational Materials Science (new, perhaps use elements from FYS-MENA4111)
5. **CS-PHYS2:** Computational Molecular dynamics in life science and materials science (new)
6. CS-KJMXXX Multi-scale molecular modeling (new course (that would be what you called **CS-PHYS2:** Computational Molecular dynamics in life science and materials science): Molecular dynamics, ab initio MD, parameterized H, Coarse grained modeling, enhanced sampling etc. . .
7. CS-KJMXXX Advanced course in Electronic structure (new course): TBD (Depends on how the KJM program develops)

Graduate Certificates. The program plans to offer graduate certificates in

- Three of the courses with label CS-MATH gives a certificate in Computational Mathematics
- Three of the courses with label CS-PHYS gives a certificate in Computational Physics, Astrophysics, Chemistry, Materials Science and Geoscience
- Three of the courses with label CS-BIO gives a certificate in Computational life science.
- Three of the courses with label CS-INF gives a certificate in High-performance computing.

Dual Degrees. The program plans to offer dual degrees (more text to come)

Description of learning outcomes

The power of the scientific method lies in identifying a given problem as a special case of an abstract class of problems, identifying general solution methods for this class of problems, and applying a general method to the specific problem (applying means, in the case of computing, calculations by pen and paper, symbolic computing, or numerical computing by ready-made and/or self-written software). This generic view on problems and methods is particularly important for understanding how to apply available, generic software to solve a particular problem.

Computing competence represents a central element in scientific problem solving, from basic education and research to essentially almost all advanced problems in modern societies. Computing competence is simply central to further progress. It enlarges the body of tools available to students and scientists beyond classical tools and allows for a more generic handling of problems. Focusing on algorithmic aspects results in deeper insights about scientific problems.

The learning outcomes are subdivided in three general categories, knowledge, skills and general competence.

- **Knowledge:** A candidate from this program
 - has deep knowledge of the scientific method and computational science at an advanced level, meaning that the candidate
 1. has the ability to understand advanced scientific results in new fields
 2. has fundamental understanding of methods and tools
 3. can develop and apply advanced computational methods to scientific problems
 4. is capable of judging and analyzing all parts of the obtained scientific results

5. can present results orally and in written form as scientific reports/articles
 6. can propose new hypotheses and suggest solution paths
 7. can generalize mathematical algorithms and apply them to new situations
 8. can link computational models to specific applications and/or experimental data
 9. can develop models and algorithms to describe experimental data
 10. masters methods for reproducibility and how to link this to a sound ethical scientific conduct
 11. has a thorough understanding of how computing is used to solve scientific problems
 12. knows fundamental algorithms in computational science
- has a fundamental understanding and knowledge of scientific work, meaning that
 1. the candidate can develop hypotheses and suggest ways to test these
 2. can use relevant analytical, experimental and numerical tools and results to test the scientific hypotheses
 3. can generalize from numerical and experimental data to mathematical models and underlying principles
 4. can analyze the results and evaluate their relevance with respect to the actual problems and/or hypotheses
 5. can present the results according to good scientific practices
- **Skills:** A candidate from this program
 - has a deep understanding of what computing means, entailing several or all of the topics listed below
 1. knows the most fundamental algorithms involved, how to optimize these and perform statistical uncertainty quantification
 2. has overview of advanced algorithms and how they can be accessed in available software and how they are used to solve scientific problems
 3. has knowledge and understands high-performance computing elements: memory usage, vectorization and parallel algorithms
 4. can use efficiently high-performance computing resources, from compilers to hardware architectures
 5. understands approximation errors and what can go wrong with algorithms
 6. has knowledge of at least one computer algebra system and how it is applied to perform classical mathematics

7. has extensive experience with programming in a high-level language (MATLAB, Python, R)
8. has experience with programming in a compiled language (Fortran, C, C++)
9. has experience with implementing and applying numerical algorithms in reusable software that acknowledges the generic nature of the mathematical algorithms
10. has experience with debugging software
11. has experience with test frameworks and procedures
12. has experience with different visualization techniques for different types of data
13. can critically evaluate results and errors
14. can develop algorithms and software for complicated scientific problems independently and in collaboration with other students
15. masters software carpentry: can design a maintainable program in a systematic way, use version control systems, and write scripts to automate manual work
16. understands how to increase the efficiency of numerical algorithms and pertinent software
17. has knowledge of stringent requirements to efficiency and precision of software
18. understands tools to make science reproducible and has a sound ethical approach to scientific problems

- **General competence:** A candidate from this program

- is able to develop professional competence through the thesis work, entailing:
 1. mature professionally and be able to work independently
 2. can communicate in a professional way scientific results, orally and in written form
 3. can plan and complete a research project
 4. can develop a scientific intuition and understanding that makes it possible to present and discuss scientific problems, results and uncertainties
- is able to develop virtues, values and attitudes that lead to a better understanding of ethical aspects of the scientific method, as well as promoting central aspects of the scientific method to society. This means for example that the candidate
 1. can reflect on and develop strategies for making science reproducible and to promote the need for a proper ethical conduct
 2. has a deep understanding of the role basic and applied research and computing play for progress in society

3. is able to promote, use and develop version control tools in order to make science reproducible
4. is able to critically evaluate the consequences of own research and how this impacts society
5. matures an understanding of the links between basic and applied research and how these shape, in a fundamental way, progress in science and technology
6. can develop an understanding of the role research and science can play together with industry and society in general
7. can reflect over and develop learning strategies for life-long learning.

By completing a Master of Science thesis, the candidate will have developed a critical understanding of the scientific methods which have been studied, has a better understanding of the scientific process per se as well as having developed perspectives for future work and how to verify and validate scientific results.

Admission criteria: Chemistry

The program has a minimum course requirement of 120 ECTS (European Credit Transfer System) at the undergraduate level (bachelor degree or equivalent) in Astrophysics, bioscience, chemistry, computer science and informatics, geoscience, mathematics, materials science, mechanics and physics.

1. Of these 120 ECTS, 40 ECTS have to include basic mathematics and programming courses, equivalent to the University of Oslo mathematics courses MAT1100, MAT1110, MAT1120, MAT1050 and MAT1060 and at least one of the corresponding computing and programming courses INF1000/INF1110 or MAT-INF1100/MAT-INF1100L/BIOS1100/KJM-INF1xxx/GEO-KJM1040.
2. The remaining 80 ECTS have to be within at most two of the fields of astrophysics, bioscience, chemistry, computer science and informatics, geoscience, mathematics, materials science, mechanics and physics. 40 of these 80 ECTS have to be advanced undergraduate courses at the 2000 and 3000 level and a minimum of 20 ECTS must be at the 3000 level within physics/material science/mechanics/astrophysics/informatics/mathematics/bioscience/chemistry/geoscience.
3. An average mark C (European grading scale) is required for the 40 ECTS in mathematics and programming (corresponding to the University of Oslo courses MAT1100, MAT1110, MAT1120, MAT1050 and MAT1060 and the corresponding computing and programming courses INF1000/INF1110 or MAT-INF1100/MAT-INF1100L/BIOS1100/KJM-INF1xxx/GEO-KJM1040 or similar courses) and the 40 ECTS at the 2000 and 3000 level. A minimum of 20 ECTS must be at the 3000 level within physics/material science/mechanics/astrophysics/mechanics/mathematics/informatics/bioscience/chemistry/geoscience.

Study abroad and international collaborators

Students at the University of Oslo may choose to [take parts of their degrees at a university abroad](#). The University of Oslo has exchange agreements with other universities in different parts of the world. [The MN Faculty has additional exchange agreements with many universities abroad](#).

Students in this program have a number of interesting international exchange possibilities. The involved researchers have extensive collaborations with: **add text**

Career prospects

Candidates who are capable of modeling and understanding complicated systems in natural science, are in short supply in society. The computational methods and approaches to scientific problems students learn when working on their thesis projects are very similar to the methods they will use in later stages of their careers. To handle large numerical projects demands structured thinking and good analytical skills and a thorough understanding of the problems to be solved. This knowledge makes the students unique on the labor market.

Career opportunities are many, from research institutes, universities and university colleges and a multitude of companies. Examples include IBM, Hydro, Statoil, and Telenor. The program gives an excellent background for further studies, with a PhD as one possible goal.

The program has also a strong international element which allows students to gain important experience from international collaborations in science, with the opportunity to spend parts of the time spent on thesis work at research institutions abroad.