Master program in Computational Science at the University of Oslo

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Planned start: Fall 2018

Master program in Computational Science

We propose a new Master of Science program at the Faculty of Mathematics and Natural Sciences of the University of Oslo. This program is called **Computational Science**, with acronym **CS**

The program is a collaboration between six departments and classical disciplines:

- Institute of Theoretical Astrophysics
- Department of Biosciences
- Department of Chemistry
- Department of Informatics
- Department of Mathematics
- Department of Physics

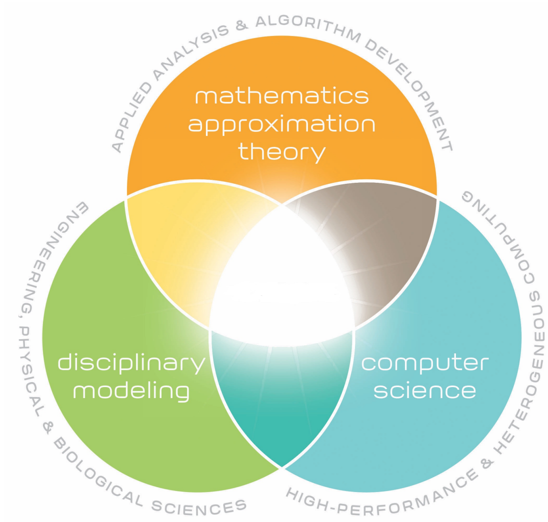
The program will be administrated by the Department of Physics.

The program is multidisciplinary and all students who have completed undergraduate studies in science and engineering, with a sufficient quantitative background, are eligible. The language of instruction is English.

Strategic importance

The program will educate the next generation of cross-disciplinary science students with the knowledge, skills, and values needed to pose and solve current and new scientific, technological and societal challenges. The program will lay the foundation for cross-disciplinary educational, research and innovation activities.

It is the first educational program to comprehensively treat computation as the *triple junction* of algorithm development and analysis, high performance computing, and applications to scientific and engineering modeling and data science. This approach recognizes computation as a new discipline rather than being decentralized into isolated sub-disciplines. The CS program will will enable application-driven computational modeling while also exposing disciplinary computational scientists to advanced tools and techniques, which will ignite new transformational connections in research and education.



Vision for the future: Scientific Computing and Data Science

Scientific computing focuses on the development of predictive computer models of the world around us. As study of physical phenomena through experimentation has become impossible, impractical and/or expensive, computational modeling has become the primary tool for understanding—equal in stature to analysis and experiment. The discipline of scientific computing is the development of new methods that make challenging problems tractable on modern computing platforms, providing scientists and engineers with key windows into the world around us.

Data science focuses on the development of tools designed to find trends within datasets that help scientists who are challenged with massive amounts of data to assess key relations within those datasets. These key relations provide hooks that allow scientists to identify models which, in turn, facilitate making accurate predictions in complex systems. For example, a key data science goal on the biological side would be better care for patients (e.g., personalized medicine). Given a patient's genetic makeup, the proper data-driven model would identify the most effective treatment for that patient.

Aims of the program

A specific aim of this program is to develop the students' ability to pose and solve problems that combine physical insights with mathematical tools and computational skills. This provides a unique combination of applied and theoretical knowledge and skills. These features are invaluable for the development of multi-disciplinary educational and research programs. The main focus is not to educate computer specialists, but to educate students with a solid understanding in basic science as well as an integrated knowledge on how to use essential methods from computational science. This requires an education that covers both the specific disciplines like physics, biology, geoscience, mathematics etc with a strong background in computational science.

A significant aspect of this program is the ability to offer new educational opportunities that are aligned with the needs of a 21st century workforce. Many companies are seeking individuals who have knowledge of both a specific discipline and computational modeling.

We plan to offer first Master of Science degrees in Computational Science and our students will be expressly educated in the use of computing to model and study the world around them. Students in the CS program will achieve a high degree of proficiency in model development, critical thinking and analysis.

Scientific and educational motivation

Applications of simulation. Numerical simulations of various systems in science are central to our basic understanding of nature and technlogy. The increase in computational power, improved algorithms for solving problems in science as well as access to high-performance facilities, allow researchers nowadays to study complicated systems across many length and energy scales. Applications span from studying quantum physical systems in nanotechnology and the characteristics of new materials or subamotic physics at its smallest length scale, to simulating galaxies and the evolution of the universe. In between, simulations are key to understanding cancer treatment and how the brain works, predicting climate changes and this week's weather, simulating natural disasters, semi-conductor devices, quantum computers, as well as assessing risk in the insurance and financial industry. These are just a few topics already well covered at the University of Oslo and that can be topics for coming thesis projects as well as research directions.

Job market. A large number of the candidates from the five involved departments get jobs where numerical simulations are central and essential. The proposed program will raise the educational quality in this area, because our candidates need a broader understanding of the possibilities and limitations of computation-based problem solving.

Multiscale modeling is a big open research question

Today's problems, unlike traditional science and engineering, involve complex systems with many distinct physical processes. The wide open research topic of this century, both in industry and at universities, is how to effectively couple processes across different length and energy scales. Progress will rely on a multi-disciplinary approach and therefore a need for a multi-disciplinary educational program.

The proposed program will foster candidates with the right multi-disciplinary background and computational thinking for understanding today's simulation technology and its challenges.

The new program combines old and new initiatives

This program builds on the strengths and successes of two existing Master of Science directions at the University of Oslo, namely the programs in Computational Physics (at the Dept. of Physics) and Applied Mathematics and Mechanics (at the Dept. of Mathematics). These programs were established in 2003. Based on the experience from these programs, the hope is that the proposed program can enlarge the reach of disciplines where computations play and/or are expected to play a large. In particular, new directions in Computational Life Science need to be developed to meet coming needs of the scientific community. We believe this new direction is best developed in close collaboration with already successful computational science programs.

Computational Physics at UiO has been a great success

This initiative has its roots in the highly successful direction called Computational Physics under the Master program in Physics at the University of Oslo.

This program has educated almost 60 Master of Science students during the last ten years. Over 50% of these students have continued with PhD studies in Physics, Chemistry, Mathematics and now recently Biology connected with the CINPLA project.

The Computational Physics Master program received in 2015 the University of Oslo Educational Award.

The new program will also host the CSE project

The new proposed program will also take a leading responsibility in further developments of the highly successful Computing in Science Education initiative at UiO. Master of science thesis projects linked up to the CSE project will be offered.

If the program becomes successful, it will naturally lead to new cross-disciplinary research and a need for a new department in computational science.

Computing competence

Computing means solving scientific problems using computers. It covers numerical as well as symbolic computing. Computing is also about developing an understanding of the scientific process by enhancing algorithmic thinking when solving problems. Computing competence has always been a central part of the science and engineering education.

Modern computing competence is about

- derivation, verification, and implementation of algorithms
- understanding what can go wrong with algorithms
- overview of important, known algorithms
- understanding how algorithms are used to solve mathematical problems
- reproducible science and ethics
- algorithmic thinking for gaining deeper insights about scientific problems

Key elements in computing competence

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.

Today's projects in science and industry tend to involve larger teams. Tools for reliable collaboration must therefore be mastered (e.g., version control systems, automated computer experiments for reproducibility, software and method documentation).

Overarching description of the CS program

Students of this program learn to use the computer as a laboratory for solving problems in science and engineering. The program offers exciting thesis projects from many disciplines: biology and life science, chemistry, mathematics, informatics, physics, geophysics, mechanics, geology, computational finance, computational informatics, b ig data analysis, digital signal processing and image analysis – the candidates select research field according to their interests.

A Master's degree from this program gives the candidate a methodical training in planning, conducting, and reporting large research projects, often together with other students and university teachers. THe projects emphasize finding practical solutions, developing an intuitive understanding of the science and the scientific methods needed to solve complicated problems, use of many tools, and not least developing own creativity and independent thinking. The thesis work is a scientific project where the candidates learn to tackle a scientific problem in a professional manner. The program aims also at developing a deep understanding of the role of computing in solving modern scientific problems. A candidate from this program gains deep insights in the fundamnetal role computations play in our advancement of science and technology, as well as the role computations play in society.

Description of learning outcomes

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A candidate with a Master of Science degree 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 scienfitic conduct

- has a fundamental understanding 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

- has a deep understanding of what computing means, entailing several or all of the topics listed below

    1. has a thorough understanding of how computing is used to solve scientific problems
    2. knows the most fundamental algorithms involved, how to optimize these and perform statistical uncertainty quantification
    3. has overview of advanced algorithms and how they can be accessed in available software and how they are used to solve scientific problems
    4. has knowledge of high-performance computing elements: memory usage, vectorization and parallel algorithms
    5. can use effeciently high-performance computing resources, from compilers to hardware architectures
    6. understands approximation errors and what can go wrong with algorithms
    7. has knowledge of at least one computer algebra system and how it is applied to perform classical mathematics
    8. has extensive experience with programming in a high-level language (MATLAB, Python, R)
    9. has experience with programming in a compiled language (Fortran, C, C++)
    10. has experience with implementing and applying numerical algorithms in reusable software that acknowledges the generic nature of the mathematical algorithms
    11. has experience with debugging software
    12. has experience with test frameworks and procedures
    13. has experience with different visualization techniques for different types of data
    14. can critically evaluate results and errors

15. can develop algorithms and software for complicated scientific problems independently and in collaboration with other students
16. masters software carpentry: can design a maintainable program in a systematic way, use version control systems, and write scripts to automate manual work
17. understands how to increase the efficiency of numerical algorithms and pertinent software
18. has knowledge of stringent requirements to efficiency and precision of software
19. understands tools to make science reproducible and has a sound ethical approach to scientific problems

- 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 maakes 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 understading 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 critera

The following higher education entrance qualifications are needed

- A completed bachelor's degree (undergraduate) comparable to a Norwegian bachelor's degree in one of the following disciplines

    1. Biology, molecular biology, biochemistry or any life science degree
    2. Physics, astrophysics, astronomy, geophysics and meteorology
    3. Mathematics, mechanics, statistics and computational mathematics
    4. Computer science and electronics
    5. Chemistry
    6. Materials Science and nanotechnology
    7. Any undergraduate degree in engineering
    8. Mathematical finance and economy
    9. Economy

- For international students, an internationally recognised English language proficiency test is required.

The above undergraduate degrees have some minimal requirements on specializations which need to be fulfilled. In addition to the above required undergraduate degrees, students need to have 40 ECTS in basic undergraduate mathematics and programming courses (calculus, linear algebra and/or mathematical modeling and programming). A course in programming is compulsory and should correspond at least to 10 ECTS of work load. The average mark for the mathematics and programming courses, as well as 40 ECTS in senior undergraduate courses (2000 and 3000 level in Norway) for the specific specialization has at least to be C (letter marks). As an example, an undergraduate degree in Chemistry has a minimal requirement on chemistry courses, typically amounting to at least 60 ECTS out of 180 ECTS for a bachelor's degree. The average mark on the 40 ECTS of selected senior undergraduate credits in chemistry and the 40 ECTS in mathematics and programming should at least be C. **A letter of motivation and two letters of recommendation are required when applying**.

Thesis directions

The program aims at offering thesis projects in a variety of fields. The scientists involved in this program can offer thesis topics that cover several disciplines. These are

- Computational Science: Astrophysics
- Computational Science: Bioscience
- Computational Science: Chemistry
- Computational Science: Finance and Risk Analysis
- Computational Science: Imaging and Biomedical Computing
- Computational Science: Materials science
- Computational Science: Mathematics
- Computational Science: Mechanics
- Computational Science: Physics

The thesis projects will be tailored to the student's needs, wishes and scientific background. The projects can easily incorporate topics from more than one discipline.

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

The 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, avoding thereby the limitation of 10 ECTS per course only. Some of these courses are listed below.

Required courses

In order to build a common study program and identity as a Computational Science student, there will be two compulsory courses that aim at providing topics of common and broad interest. Both courses have a workload of 10 ECTS each. The courses are

- **CS1**: *High-Performance Computing and Numerical projects*, 10 ECTS

1. This course teaches you to develop and structure large numerical projects, from code writing to finalizing a report
2. Topics which are included are parallelization and vectorization (based on INF3380)
3. Machine architecture and GPU-CPU programming
4. Optimization of code and benchmarking
5. Numerical methods from linear algebra will be discussed as well as examples from life science.

- **CS2**: *Data analysis and machine learning*, 10 ECTS

1. Monte Carlo methods and statistical data analysis
2. Optimization of data and handling of large data sets
3. Machine learning and neural networks

Presently available courses at UiO and NMBU

The program aims at reorganizing many of the existing courses. Here follows a list of suggested courses that students may include in their required course load.

- FYS4150 Computational Physics I
- FYS4411 Computational Physics II
- FYS4460 Computational Physics III
- INF5620 Numerical Methods for Partial Differential Equations
- INF5631 Project on Numerical Methods for Partial Differential Equations
- FYS388 Computational Neuroscience
- STK4520 Laboratory for Finance and Insurance Mathematics
- STK4021 Applied Bayesian Analysis and Numerical Methods
- MAT-INF4130 Numerical Linear Algebra
- MAT-INF4110 Mathematical Optimization
- ECON4240 Equilibrium, welfare and information
- MEK4470 Computational Fluid Mechanics
- MEK4250 Finite Element Methods in Computational Mechanics
- AST5210 Stellar Atmospheres I

- AST9110 Numerical Modeling

The program plans to develop other courses in computational science and its applications, ranging from life science to materials science. Courses on project planning and project administration are also possible to include.

Possible new courses

Some of these courses could incorporate (or base themselves upon) existing ones

- **CS3**: Basic methods in computational modeling
- **CS4**: Mathematical Foundations of data science (based on MAT-INF4110 and STK4021)
- **CS5**: Computational Linear Algebra (based on MAT-INF4130)
- **CS6**: Computational differential equations (Based on INF5620)
- **CS7**: Computational Bioinformatics (Based on INF5380)
- **CS8**: Molecular dynamics in life science and materials science
- **CS9**: Advanced optimization of numerical code (follows up CS1)
- **CS10**: Computational Astrophysics (based on AST9110)
- **CS11**: Computational quantum mechanics (based on fys4411 and FYS-MENA4110)
- **CS12**: Computational statistical mechanics (based on fys4460)
- **CS13**: Computational finance (based on STK4520)
- **CS14**: Advanced data science
- **CS15**: Computational Mechanics (based on MEK4470 and MEK4250?)

Graduate Certificates

The program plans to offer raduate certificates in

- Computational Modeling for those studens who take 30 ECTS in modeling courses
- High-performance computing for those studens who take 30 ECTS in high-performance computing

The program opens up for flexible backgrounds

While discipline-based master's programs tend to introduce very strict requirements to courses, we believe in adapting a computational thesis topic to the student's background, thereby opening up for students with a wide range of bachelor's degrees. A very heterogeneous student community is thought to be a strength and unique feature of this program.

Study abroad and international collaborators

Students at the University of Oslo may choose to take parts of their degrees at a university abroad.

Students in this program have a number of interesting international exchange possibilities. The involved researchers have extensive collaborations with other researchers worldwide. These exchange possibility range from top universities in the USA, Asia and Europe as well as leading National Laboratories in the USA.

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.

Dual master degrees

More material to come. Several places offer this path..