Master program in Computational Science at the University of Oslo

Tom Andersen¹

Andreas Austeng²

Arne Bang Huseby³

John Burkart⁴

Michele Cascella 5

 ${\bf Mats~Carlsson}^6$

 $Geir Dahl^3$

Simon Wolfgang Funke^{2,7}

Marianne Fyhn¹

Viggo Hansteen⁶

Morten Hjorth-Jensen (chair)⁸

Joseph Lacasce⁴

Katrine Langvad (admin)⁸

Anders Malthe-Sørenssen⁸

Kend-Andre Mardal³

Martin Reimers³

Knut Mørken³

Torbjørn Rognes²

Thomas Schuler 4

Grete Stavik-Døvle (admin)⁸

 ${\bf Joakim~Sundnes}^{2,7}$

¹Department of Biosciences, University of Oslo
²Department of Informatics, University of Oslo
³Department of Mathematics, University of Oslo
⁴Department of Geoscience, University of Oslo
⁵Department of Chemistry, University of Oslo
⁶Institute for Theoretical Astrophysics, University of Oslo
⁷Simula Research Laboratory
⁸Department of Physics, University of Oslo

Planned start: Fall 2018

Master program in Computational Science

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

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

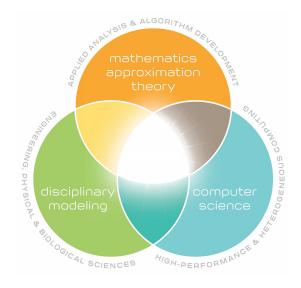
The program is multidisciplinary and all students who have completed undergraduate studies in science and engineering, with a sufficient quantitative background, are eligible.

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 enable applicationdriven computational modeling while also exposing disciplinary computational scientists to advanced tools and techniques, which will ignite new transformational connections in research and education.



The new program and 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. For future discussions: how to link with CCSE.

If the program becomes successful, it will naturally lead to new cross-disciplinary research. And perhaps for a new department in computational science!! Back to Hans Petter slides from 2005.

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: Biology and Bioinformatics

• Computational Science: Chemistry

• Computational Science: Finance and Risk Analysis

• Computational Science: Geoscience

• Computational Science: Imaging and Biomedical Computing

• Computational Science: Materials science

• Computational Science: Mathematics

• Computational Science: Mechanics

• Computational Science: Physics

• Wish: Computational Science: Economy and finance

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.

Required courses

In order to build a common study program and identity as a Computational Science student, we plan be two compulsory courses that aim at providing topics of common and broad interest.

- CS-MATH1: Data analysis and machine learning, 10 ECTS (Existing ST2100, GEO4330)
 - 1. Monte Carlo methods and statistical data analysis
 - 2. Optimization of data and handling of large data sets
 - 3. Machine learning and neural networks
- CS-INF1: High-Performance Computing and Numerical projects, 10 ECTS (Existing INF3380)
 - 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
 - 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.

Presently available courses at UiO and NMBU (not exhaustive)

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
- GEO4330 Advanced hydrological modelling
- AST5210 Stellar Atmospheres I
- AST9110 Numerical Modeling

Possible new courses

Some of these courses could incorporate (or base themselves upon) existing ones. The courses here are organized according to their corresponding disciplines.

- Mathematics
 - CS-MATH1: Data analysis and machine learning (Existing GEO4330, STK2100)
 - 2. **CS-MATH2**: Basic methods in computational modeling (new? do we need it?)

- 3. **CS-MATH3**: Mathematical Foundations of data science (based on MAT-INF4110 and STK4021)
- 4. CS-MATH4: Computational Linear Algebra (based on MAT-INF4130)
- 5. **CS-MATH5**: Computational differential equations (Based on INF5620)
- 6. **CS-MATH6**: Computational finance (based on STK4520)
- 7. **CS-MATH7**: Advanced data science (new)
- Physical sciences (Astrophysics, geoscience, physics, chemistry and materials science)
 - 1. CS-PHYS1: Computational Physics (based on FYS3150/4150)
 - 2. **CS-PHYS2**: Molecular dynamics in life science and materials science (new)
 - 3. CS-PHYS3: Computational Astrophysics (based on AST9110)
 - 4. **CS-PHYS4**: Computational quantum mechanics (based on fys4411 and FYS-MENA4110)
 - 5. **CS-PHYS5**: Computational statistical mechanics (based on fys4460)
 - 6. CS-PHYS6: Computational Materials Science (based on FYS-MENA4111)

• Bioscience

- 1. **CS-BIO1**: Computational Bioinformatics (Based on INF5380)
- 2. **CS-BIO2**: Advanced bioinformatics (new)
- 3. **CS-PHYS2**: Molecular dynamics in life science and materials science (new)

• Computer science

- 1. **CS-INF1**: High-Performance Computing and Numerical projects (parts of inf3380, else new)
- 2. **CS-INF2**: Advanced optimization of numerical code (new)

• Mechanics

- CS-MECH1: Computational Mechanics (based on MEK4470 and MEK4250?)
- 2. **CS-MECH2**: Advanced Computational Mechanics (new?)

Double degrees: Some observations

From Brian O'Shea, Department of Computational Mathematics, Science and Engineering, Michigan State University. ...Hi folks,

A substantial number of current nuclear theory grad students are thinking about pursuing a dual PhD in CMSE, and it seems that it's becoming a useful recruiting tool elsewhere in the physics department. I suspect it will be useful for nuclear theory as well. To that end, a description of the CMSE PhD program, which is useful for explaining the value of a dual PhD, can be found here

And a description of the dual PhD can be found here.....

Double Master degree

- A typical Computational Physics student (now) writes a Masster thesis with a mix of theoretical physics (also with analysis of experimental data) and Computational science topics.
 - This is probably the case in all other fields and makes our education and candidates attractive in the labor market.
- Set up detailed rules for double degrees, adding for example additional courses.

Graduate Certificates, several possibilities

Offer graduate certificates in

- Three of the courses with label CS-MATH gives a certificate in Computational Modeling
- 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.

Further plans when established

- Erasmus+, excellent opportunity to build up an international Master of Science program in Computational Science, with stipends to studens from non-European countries
- Doctoral school (national) and Marie Curie graduate training program in Computational Science

- Close ties with CCSE in the beginning, but long term plan is a new Department of Computational Science
 - An excellent example is the new Department of Computational Mathematics, Science and Engineering at Michigan State University
 - * 30 new positions, many of these shared with other departments
 - * Undergraduate programs, from minor to major degrees
 - $\ast\,$ Graduate programs, MSc and PhD, dual degrees
 - $\ast\,$ new educational programs, but our new CS program is broader
 - Many similar departments in Northern America but few in Europe.