Computing Across the Disciplines (CAD): How UiO should meet the Future

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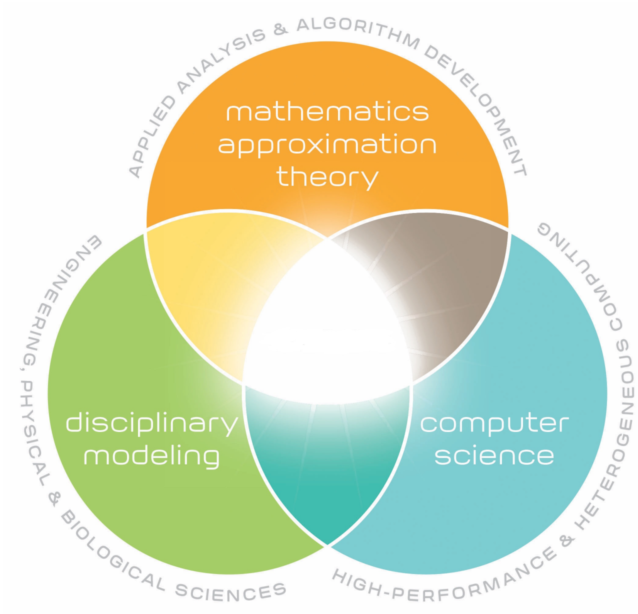
A whitepaper on how to organize Computational Science and Data Science initiatives at UiO, prepared for the Mat-Nat Fakultetet of the University of Oslo

Executive Summary

This proposal seeks to transform the University of Oslo (UiO) to become a leader nationally and internationally in scientific discovery through large-scale computations and data-driven research. The aim is to position UiO as a leader in computational and data sciences by recruiting faculty whose expertise pertains to large-scale computing and mathematical foundations of data science - both generalists (algorithm/tool developers) and specialists (focused on specific disciplines).

Modern scientists increasingly rely on computational modeling and data analysis to explore and understand the natural world. Given the ubiquitous use in research and education and its critical importance for societal development, computational science and data science play a central role in progress and scientific developments in the 21st Century. This document aims at developing strategies for meeting these future challenges. One important step in order to meet the future, is the hiring of new researchers and faculty with the competences and skills which are needed in order to harness the many new possibilities, as well as developing new research and educational strategies that can serve our society at large.



There are several possible ways to meet these challenges and the present document offers an analysis of some of these. The present version of the document focuses on the establishment of a new department.

Other possibilities that will be explored are:

1. The establishment of one or more centers in Computational Science and Data Science. The center(s) will lay the foundation for cross-disciplinary activities and establish the necessary foundations and preparations for launching for example a new department. It will develop research projects across disciplines as well as develop educational programs and initatives related to the establishment of an eventual new department or modification of existing departments.

2. A cluster hire at various departments in order to strengthen overall research and educational competences in computational science and data science. The center could coordinate such activities or alternatively the new department. Here one could think of for example 3-5 new positions in Computational Mathematics at the Department of Mathematics, a similar amount in Physics, Bioscience, Geoscience, Economy, Social Science etc.;

3. The enlargement/change/extension of existing departments. As an example, the present Department of Mathematics could be enlarged in order to accomodate the future needs.

Irrespective of ways of organizing these activities, the university of Oslo will need to hire at least some 25-30 new faculty in order to meet future challenges.

Many of the needed competences and research area are only weakly covered, or are non-existing, by present faculty.

We propose thus a two-step process

- Establish a working group by April 1 2018. This working group will be tasked to deliver a final report with various strategies by the end of fall 2018.
- From spring 2019, start the work needed to establish for example a new Department (or center), called **Department of Computational and Data Sciences** by fall 2020. This department could be colocalized with the new center on life sciences and thus spur the development of computations in the life sciences. The new department will be a hub for innovative thinking and pave the way for research and education in computational and data science across all disciplines.

The new department and the center as well will be part of the Matematisk Naturvitenskapelige Fakultetet (MNFak in brief) of the university of Oslo, although it aims at becoming a true inter-disciplinary department serving all colleges (Law, Natural Science and Mathematics, Medicine, the Humanities, Education and the Social Sciences). It is the MNFak which will propose to the board of the university of Oslo the establishment of both the center and the department. We propose thus

1. a new Department of Computational and Data Sciences (CDS) that is administered by the MNFak and meant to facilitate interdisciplinary science by fall 2020;
2. the injection of 25-30 new faculty focusing on the science of computational modeling and data science;
3. the foundation for developing joint cutting-edge graduate and undergraduate programs.

The new faculty will thus be tasked with developing new research and educational programs in Computational Science and Data Science. The hired faculty can/will have shared positions with existing departments (for example a 70% position at the CDS department and 30% at the department of Physics), similarly, faculty with a computational profile and interest at existing departments can have shared positions at the new department. This will ensure transfer of knowledge as well as the establishment of new and cross-disciplinary research and oversee the development of new educational programs and efforts. A center solution cannot ensure the long-term sustainability of all these activities. A single department will also not be able to oversee the truly at large cross-disciplinary foundation of Computational Science and Data Science.

These efforts will open doors to new scientific challenges, will enable UiO to compete and propose new Center-level funding opportunities as well as totally new research areas (in the Humanities for example) in computation and data-driven related areas that are currently beyond our reach. It will facilitate the training of scientists and students to be an effective 21st century workforce. It will also develop courses on modern computational techniques and data modeling that meet the needs of society, both for the public and the private sector. The metrics for success are as follows. Within 5 years (2020-2025), we will have hired 25-30 world leading faculty that form the backbone of this department, who will bring in single-PI grants and small-scale (few-PI) collaborative grants, building the foundation for CDS to develop large-scale funding.

We have already developed (starting fall 2018) two new Master of Science programs, one in Computational Science which includes almost all disciplines at the MNFak and one on Data Science. These programs form the basis for our educational efforts that will lead to an **across the disciplines PhD program** serving the whole university. The PhD program will start fall 2020 when the first students from our two Master of Science program have finalized their theses. Based on the two exisiting MSc programs, the new department will research the possibilities of establishing similar MSc programs in Computation and Data Sciences for other disciplines. Similarly, the new department will aim at establishing similar programs for outside users.

The new department will coordinate many of its educational activities with the newly established center of excellence in education, the Center for Computing in Science Education. It will give the Computing in Science Education initiative a formal institutional basis and together with the Center for Computing in Science Education it will form a unique powerhouse in educational transformations. The new department will

1. Develop a comprehensive set of courses and degree programs at both undergraduate and graduate levels that will give students across the university exposure to practical computational methods, understanding how to analyse data and more generally to the idea of computers as problem-solving tools. The department will also develop Software Carpentry and Data Carpentry courses. The courses and the degree programs can also be offered as intensive training courses and programs.

2. Facilitate the adoption of computational tools and techniques for both research and education across campus, through education and faculty collaboration. A center and then a department will facilitate the pursuit of these goals!

3. Develop an all university PhD program in Computational Science and Data Science.

4. Based on the new programs (start fall 2018) on Computational Science and Data Sciece, Develop an all university Master of Science Program in Computational Science and Data Science.

5. Develop courses and course modules in Computational Science and Data Science for the private and the public sectors.

6. Develop a Master of Science program and a PhD program in Computational Science and Data Science tailored to the needs of the private and the public sectors, allowing for students residing outside UiO to develop their knowledge about Computational Science and Data Science.

7. Be a driving force in the education of the next generation of school teachers and university teachers, with a strong focus on digital competences.

Finally, this department will facilitate the growth of the university by participating in cross-cutting efforts such as the upcoming life science initiative. Within 10 years, the initiative will have secured Center-level funding via for example the Norwegian SFF system and the EU. The department will also have fully developed our graduate and undergraduate curriculae with the addition of Bachelor's programs in computational modeling and data science, and will have strong enrollment numbers in all education programs.

The new CDS department will be unique among computational academic units nationally, the first to comprehensively treat computation as the triple point of algorithm development and analysis, high performance computing, and disciplinary knowledge with applications to scientific and engineering modeling and data science. There is no such department in Norway and very few ones in Europe and Northern America. The above paradigm shift recognizes computation as a new discipline rather than decomposed into isolated sub-disciplines, enabling application-driven computational modeling and data-driven discoveries, while also exposing disciplinary computationalists to advanced tools and techniques, which will ignite new transformational connections in research and education. This research nexus also gives rise to the educational opportunities driven by similar synergy, leveraging common resources among disciplines, and enabling joint programs and unique degrees across the entire computational space.

Why should we focus on developing a department in Computational and Data Sciences?

Scientific computing plays a central role in scientific investigations and is central to innovation in most domains of our lives. It underpins the majority of today's technological, economic and societal feats and we have entered an era in which huge amounts of data offer enormous opportunities, but only to those who are able to harness them. By 2020, it is also expected that one out of every two jobs in the STEM (Science, Technology, Engineering and Mathematics) fields will be in computing (Association for Computing Machinery, 2013).

Furthermore, the 3rd Industrial Revolution will alter significantly the demands on the workforce. To adapt a highly-qualified workforce to coming challenges requires strong fundamental bases in STEM fields. Computational Science can provide such bases at all stages. Most of our students at both the undergraduate and the graduate level are unprepared to use computational modeling, data science, and high performance computing – skills valued by a very broad range of employers. The new department will also focus on the development of courses in computational science and data science tailored to the needs of the rest of society, both for the private and the public sector.

These developments, needs and future challenges, as well as the developments which are now taking place within quantum computing, quantum information and data driven discoveries (data analysis and machine learning) will play an essential role in shaping future technological developments. Most of these developments require true cross-disciplinary approaches, approaches which normally cannot be accomplished within the realms of one single disciplinary-based department.

Modern problems in science and engineering bridge a vast range of temporal and spatial scales and include a wide variety of physical processes. The analysis of such problems is not possible, so one must turn to computation. To develop computational tools for such complex systems that give physically meaningful insights requires a deep understanding of approximation theory, high performance computing, and domain specific knowledge of the area one is modeling. National laboratories like SIMULA research lab have addressed the interdisciplinary nature of computing by having experts in numerical algorithms co-located with disciplinary experts who have a deep understanding of computation, and who use scientific computing to address key topics in science.

The proposed organization with algorithmic scientists and disciplinary scientists in STEM fields as well as other fields is what facilitates the exploration of challenging multi-disciplinary and interdisciplinary topics that could not otherwise be addressed. This key observation motivates the model for the proposed department - a place where we will attack the critical problems facing us in the 21st century, problem which require the development of computing skills across disciplines, from the traditional STEM fields to the Humanities, Law, Educational Science and the Social Sciences. Furthermore, this department would strive to use computing as a critical tool to explore fundamental scientific questions in subjects as diverse as the physics of specific materials, evolutionary biology and data-driven economic forecasting. In addition, the synergy of data-driven computational modeling, combining aspects of traditional scientific computing with data science and data mining, is an exciting topic that this new unit will be uniquely suited to address. This is a rapidly emerging field that touches many of the STEM disciplines but also Medicine, Education, the Humanities and the Social Sciences, and attracting world-leading talent in this area is greatly facilitated by the introduction of the nurturing environment of the CDS department. Furthermore, the development of the Department of Computational and Data Sciences has the potential to catapult UiO into the position of being a leader in this critical new field, and will open doors to new scientific challenges as well as new Center-level funding opportunities.

To jump-start this new department at the 'triple point' of mathematics, computer science and discipline-specific computation, we propose recruiting faculty who are experts in numerical algorithms as well as those whose primary focus is the use of advanced computation to solve a wide range of challenging scientific problems. Furthermore, we wish to define scientific projects where data-driven discovery can play a major role in future years. In addition, we wish to recruit scientists - having joint appointments with other units at UiO -

whose expertise in computation on heterogeneous and/or distributed computing platforms, such as hardware-accelerated computing (e.g., GPU computing), cloud computing, and middleware for dynamic optimization across HPC architectures. To provide a critical mass, we propose hiring 25 to 30 new faculty across the aforementioned disciplines. Colocation and research and curriculum ties enable the CDS department to break down historical disciplinary boundaries, and become the synergistic leading-edge center of computational activities on campus. Furthermore, colocating these scientists will enhance the development of new computational algorithms to address pressing scientific and societal needs and enable the creation and deployment of the robust numerical tools required for the pursuit of leadership-class science in virtual laboratories. Most importantly, the new department will enable new science through these unique interdisciplinary collaborations and will become a focal point for computational research at UiO, bringing researchers in computational and data sciences together with domain experts in astrophysics, bioinformatics, chemistry, geoscience neuroscience, subatomic physics, materials science, life science, the Humanities, economy, Education and many more.

Strengths, Possibilities and Synergies. The University of Oslo has within several of the STEM fields strong research and educational activities, exemplified through for example:

- Several Centers of excellence in research where Computational Science plays a major role
- A newly established center of excellence in education research
- Newly established Master of Science programs in Computational Science and Data Science
- Several excellent groups in STEM fields that do Computational Science and Data Science
- Computational topics are included in all undergraduate STEM programs, with the possibility to develop a bachelor program in Computational Science and Data Science for all university colleges
- Several educational prizes and awards related to computational science
- Strong links with research laboratories like SIMULA research lab
- UiO has the potential to develop cross-college educational programs in Computational Science and Data Science, from undergraduate programs to PhD programs that serve also the public and the private sectors
- The courses to be developed can be offered to train employees and students outside UiO, serving thus the coming needs of for example Machine Learning for the public and the private sectors

With a center and later a department we have the possibility to really position UiO as the leading Norwegian and perhaps European institution within Computational Science and Data Science.

Enhance Computational Science and Data Science across the disciplines. Data driven discovery and data driven modeling play already a central role in research. The global objective here is to strengthen and coordinate such activities by bringing together scientists and students across the disciplines. UiO has already strong computational research and education activities within Mathematics and the Natural Sciences. The aim here is to extend this to include

- Computational Science and Data Science in Mathematics and all of the physical sciences (Astrophysics, Chemistry, Geoscience and Physics)
- Bioinformatics
- Develop research programs in Quantum Computing and Quantum Information theory. Many universities are now developing research and educational strategies in Quantum Computing
- Develop data-driven discovery research programs utilizing recent developments in machine learning
- Computational life science
- Computational Materials Science
- Computational Economy and Data Science and computing in Law and the Social Sciences
- Data Science and computing in the Humanities

The new department will host and coordinate research and educational programs in Computational Science and Data Science. In particular research and education that involve data analysis and Machine Learning will play a central role here. Similarly, the new department will be responsible for developments in quantum computing and quantum information theories.

Courses and degree programs

Creation of a robust, coherent set of undergraduate and graduate degrees, with accompanying courses, supports two complementary goals. First, a coherent program will allow the university to consolidate undergraduate and graduate training in computation in the STEM fields as well as introducing computing to other disciplines, reducing redundancy in the courses taught and allowing the university to offer a wider range of more specialized advanced courses. Second, we will create a robust set of degrees that are designed to give our students a strong introduction to computing that will complement UiO's existing disciplinary training, and which will make them better suited to be a part of the workforce in the 21st century, but also to be able to develop and use computing and data Science across the disciplines. These programs will include:

1. An undergraduate program in Computational and Data Sciences tailored to various disciplines.
2. We have already (from fall 2018) two new Master of Science programs in Computational Science and Data Science dailored to STEM fields. The aim is to extend these to other colleges.
3. Develop a cross-college PhD program in Computational Science and Data Science.
4. Develop courses and course modules in Computational Science and Data Science for the private and the public sectors.
5. Develop a Master of Science program and a PhD program in Computational Science and Data Science tailored to the needs of the private and the public sectors, allowing for participants residing outside UiO to develop their knowledge about Computational Science and Data Science.
6. Be a driving force in the education of the next generation of school teachers and university teachers, with a strong focus on digital competences.

This range of options will allow some number of students to dive deeply into computation through the degree programs, and will enable a much broader swath of the UiO population to learn about some aspects of computational and data science through not only the various programs but also through the courses to be developed by the new department.

One desired result of the creation of these courses and programs is the foundation of a strong community of students from different disciplines who use similar techniques to solve a wide range of problems, which will promote broad, interdisciplinary thinking and will help to raise the visibility of computing throughout the UiO campus. We note that an extra benefit of these educational efforts is that UiO will become an ideal place to perform research in computational science education, a topic of critical importance that has thus far received little scholarly attention. The new department will have strong links with the recently established Center for Computing in Science Education.

Long term goals and sustainability. The overall goal of this department is to bring together world-leading faculty who combine the most important aspects of computation and disciplinary research, thus enabling cutting-edge interdisciplinary science and the training of both undergraduate and graduate students. The department will be economically sustained through the standard base university funding, as any other department at Norwegian universities. However, additional funds will be realized by the securing for example Center-level funding (as well as many single- or few-PI grants), as well grants obtained the PIs that sustain graduate students, post-docs, travel and other associated expenses. In order to ensure the success of these efforts, the proposed department must be financially sustainable. Basic university funding (beyond faculty and support staff salaries) is necessary to support fellowships for top graduate students, speaker series and honoraria, visitor support, hardware purchases, and startup packages.

The enclosed appendices contain more details about the structure of the planned department, with research and education plans. Links to similar and recently established departments are also presented.

Appendix A: Tentative list of working group members (February 2018)

1. Bioscience: Tom Andersen, Marianne Fyhn and Lex Nederbragt
2. Chemistry and Hylleraas Center for Quantum Molecular Sciences: Michele Cascella
3. Geoscience: John Burkhart, Joe Lacasce and Thomas Vikhamar Schuler
4. IFI: Andreas Austeng,Xing Cai, Joakim Sundnes
5. Math: Kent-Andre Mardal and Knut Mørken
6. Physics and Center of Computing in Science Education: John Mark Aiken, Morten Hjorth-Jensen and Anders Malthe-Sørenssen
7. SIMULA research lab: Xing Cai, Simon Funke, Marie Rognes, Joakim Sundnes, and Aslak Tveito
8. Department of Political Science: Bjørn Høyland
9. Department of Sociology and Human Geography: Torkild Hovde Lyngstad
10. Department of Psychology: Nikolai Olavi Czajkowski

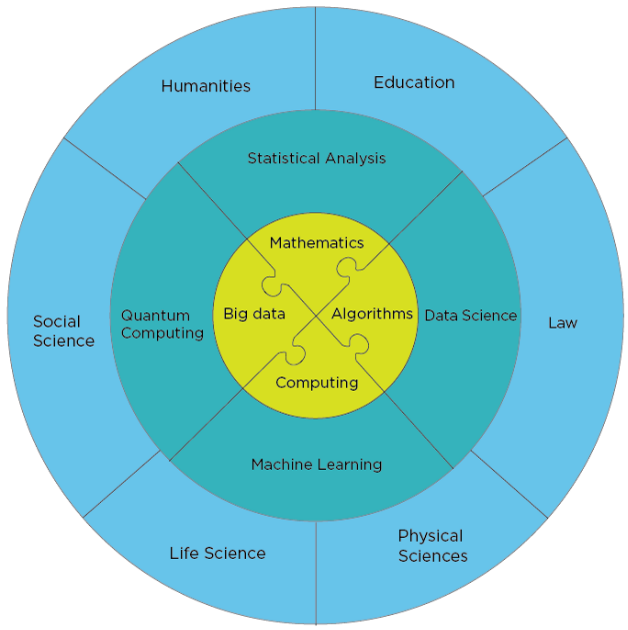
Appendix B: Structure and Justification for Planned Organization

We envision that the CDS department will be a truly interdisciplinary unit that strives to focus on algorithmic science and its applications to a range of critical research topics. The CDS department will consist of 25-30 faculty, comprising generalists and disciplinary scientists. The generalists develop cross-disciplinary tools addressing large classes of problems. The disciplinary scientists pursue model/algorithm development from a domain-specific perspective, enabling application-specific approximations and optimization of performance on exascale problems. The nexus of these groups is what makes CDS unique.

The cross-disciplinary working group that developed this proposal seeks the creation of a joint, inter-college department as the ideal solution. This structure, is necessary to facilitate the recruiting of a core group of faculty whose focus is on algorithmic science that can be applied to new scientific challenges and computational platforms. The reasoning behind this is straightforward - the fundamental science we are interested in developing is clearly growing beyond the boundaries of existing STEM disciplines, in the same way that the discipline of computer science grew beyond the boundaries of historical roots in mathematics or electrical engineering. It is advantageous to be at the forefront of this trend. This new department is at the forefront of a key paradigm shift. Discipline-focused departments tend to only place value on the new science a computer programs can explore, and to not place value on the time or energy it takes to develop critical algorithms and tools that provide a deeper understanding of fundamental processes in the various disciplines. By placing the home of computational scientists in this new department, we accomplish two critical goals. First, a single department focused on the science of computation will strengthen the goal of interdisciplinary collaboration, as faculty in this new unit will have a wide range of backgrounds in many traditional disciplines, and not only the traditional STEM disciplines. Second, the new department will break down traditional barriers between departments, as the common theme of the new department is the science of algorithms and their applications, providing a key place for critical interactions between different scientific communities. While many faculty will have full appointments in the department, joint appointments will help to cement interdepartmental collaboration and build up a strong interdisciplinary community. This gives UiO the flexibility to grow into this critical area by hiring cutting-edge interdisciplinary scientists, and will also allow existing disciplinary departments the opportunity to grow beyond their current boundaries.

The joint appointments with other departments will play an important role in cementing the structure of the CDS department, strengthening cross-disciplinarity collaborations. Furthermore, the task of developing new and joint courses will require extensive collaborations across departments. As an example, faculty hired by the new department could have a 70% appointment with the new department and 30% with a single discipline oriented department. Similarly, a researcher with linked to the department of Chemistry, could have a shared position of for example 20% at the CSD and 80% at the department of Chemistry. These joint appointments will facilitate the seeding of new research and the development of new courses and degree programs.

One can view the new department as a hub which focuses on Algorithms, Computing, Big Data, Mathematics, Quantum Computing, Machine Learning and Statistical Analysis in close collaboration with scientists working from the Physical Sciences (Chemistry, Astrophysics, Physics, Geoscience, Mechanics, Materials Science), Life Science (Bioscience and Medicine), Law, Education, Social Sciences and the Humanities. The new department will develop and strengthen the field of Computational Science and Data Science in close collaboration with all involved departments (from the MNfak and other colleges), increasing thereby the overall general competences of our students and scientific staff on these topics. The following figure illustrates schematically these links, with the two inner circles representing the most likely key research activities of the new department.



Funding. In order to secure funding in addition to those guaranteed by the University and the ministry of education and research, the department will seek assiduously center funding from the Norwegian SFF and SFI system (under the auspices of the Research Council of Norway) as well as similar funding possibilities from the EU. In addition, we expect the faculty to bring in regular research grants either from industry, the Research Council of Norway or the EU.

We aim also at exploring and having, out of the 25-30 positions, five positions at the level of associate or full professor as endowed chairs and professorships from the private sector. We will in particular target companies where computational science and data science will play a major role in the future. The design of research projects linked to the needs of these companies as well as the PhD and Master of Science programs discussed below, will make sure that both the private and the public sector will benefit from highly qualified candidates.

Below we discuss several possible research directions where faculty hires can start new research directions, in close collaborations with specialists from various departments.

Appendix C: Sampling of new and transformational science that will be enabled by the new department

There are several new and emerging research directions where the new department will play and can play a major role.

Computational life science. The Life Sciences is transforming with the explosion of High-throughput data generation technologies and the need for integrating these across all the levels of the biological hierarchy. A 'system-dynamic' (Systems Biology) approach will dominate research in the coming decades. Here, computational modelling to integrate the various data types and data sets will be a driving force. Similar developments are seen in the field of molecular image analysis, where computational methods to integrate the image streams will become essential to make sense of the growing amount of data. Translational Bioinformatics, bridging the gap between the laboratory, computer and the clinic, with the ultimate goal of personalised medicine, is an important, and exciting new dimension. Many of these developments require cross-disciplinary thinking, and often breakthroughs in Bioinformatics/Computational Life Science start with creatively adjusting and implementing algorithmic or computational solutions originally developed for other fields. A CDS department that has multidisciplinarity as its founding principle, and brings computationally skilled researchers from many fields together, will provide a solid foundation for researchers working towards these developments.

Develop data-driven discovery research programs utilizing recent developments in machine learning. **Machine Learning** plays nowadays a central role in the analysis of large data sets in order to extract information about complicated correlations. This information is often difficult to obtain with traditional methods. For example, there are about one trillion web pages; more than one hour of video is uploaded to YouTube every second, amounting to 10 years of content every day; the genomes of 1000s of people, each of which has a length of 3.0×10^9 base pairs, have been sequenced by various labs and so on. This deluge of data calls for automated methods of data analysis, which is exactly what machine learning provides. Developing activities in these frontier computational technologies is thus of strategic importance for our capability to address future science problems. The applicability of big data, data-driven discoveries, data-driven modeling and machine learning covers basically all disciplines and fields, with applications spanning from materials science, mechanics, medicine, applied mathematics, economic forecasting etc. Machine learning and big data concepts are being exploited in more and more fields. The big data challenge will be in the forefront of biology and life science research in the next few years. In materials science machine learning allows us to parametrize results from quantum mechanical calculations in terms of classical interactions. These interactions are in turn suitable for large scale molecular dynamics simulations of complicated systems spanning from subatomic physics to materials science and life science. To develop a multiscale science program starting with the smallest constituents and moving to larger systems can most likely only be done with the development and application of machine learning algorithms. Economists and policy makers need up-to-date information on the state of the economy to formulate effective policies. Variables such as GDP, Gini factors, unemployment rates, quality of life data etc are normally used as key indicators. These data are often only available with delays between collection and availiability to analysts, making it thus difficult to asses properly their relevance. Machine learning algorithms have the potential to deliver improved predictions as well as correlations and proper error estimates. The examples discussed here represent just a few of the possible applications of Machine Learning algorithms that the new department can aid in developing. To develop these research lines will be achieved most effectively within the multidisciplinary CDS department.

Develop research programs in Quantum Computing and Quantum Information theory. Enabling simulations of large-scale quantal many-particle systems is a long-standing problem in scientific computing. Quantum many-particle interactions define the structure of the universe, from nucleons and nuclei, to atoms, molecules, and even stars. Since the discovery of quantum mechanics, a lot of progress has been made in understanding the dynamics of certain many-particle systems. While some of our insight comes from a small set of analytically solvable models, numerical simulations have become a mainstay in our understanding of many-particle dynamics. The progress in numerical simulations has accelerated in the last few decades with the advent of modern high performance computing (HPC) and clever developments in classical simulation algorithms such as, quantum Monte Carlo,large-scale diagonalization approaches, Coupled-Cluster theory and other renormalization schemes. Despite the monumental advances, classical simulation techniques are reaching fundamental limits in terms of the size of the quantum systems that can be processed. Fortunately, the disruptive new field of quantum simulations has emerged, promising to enable simulations far beyond those which are classically tractable. In particular, scientific applications concerned with simulations of interacting fermions on a lattice are poised to reap the benefits of quantum simulations. Mathematical models of interacting fermions naturally extend to describe vastly different physics such as that of correlated electronic and the correlated nuclear systems.

Recent progress in quantum computing as well as digital and analog Quantum Algorithms (QAs) promise to enable the exciting possibility of performing simulations that are beyond the reach of all existing and future classical supercomputers. Despite the progress, there is still a gap between the resources required by state-of-the-art QA and the resources offered by available and near-future quantum hardware. It may take decades of quantum hardware development and engineering before the current QAs will outperform classical exascale class simulations. Therefore, to impact scientific computing on a more relevant time scale, improving the scalability and efficiency of quantum simulation algorithms is of the highest importance. Developments in quantum information algorithms and their mathematical properties, as well as their applications will play a critical role in studies of relevance for a wide variety of fields, from the design and studies of new materials to our basic understanding of systems of interest in chemistry and physics. The new department, in close collaboration with disciplinary experts, can play an essential role in developing this field by hiring world-leading experts in quantum information theory and quantum computing.

Computational Social Science. Survey data, the engine of the behavioral revolution of the social sciences is about to run its course, with low response rate and poorly representative samples being the norm rather than the exception. Fortunately, vast amount of new information from social media, via digitalized governmental archives, to population registries are opening up new exiting avenues for innovative social science research, such as paternity leave and children's performance in school, extent of censorship in Chinese online new reporting, or conditions for receptiveness to fake news. Moreover, the new data availability in combination with tools from machine-learning has spurred an interest in prediction and sophisticated policy-recommendations, ranging from optimize relocation of immigrants given their skill-set and local labor market needs, via probabilistic detection of election fraud, to forecasting of popular unrest and civil war. The undertaking of such research questions was, until recently, outside the realm of social science. There are however limits to the amount of new insights that can be obtained purely from richer data and "black-box" import of machine-learning tools. More robust, new insights require similar steps to be taken in the development of applied, testable, theoretical models to facilitate direct empirical evaluations of the model dynamics and the consistency of the model with the data. Such a step requires a solid grounding in computing.

Computational Geoscience. Geoscience has long been a computationally-intensive area. A typical climate simulation, used for example in the future projections discussed by the Intergovernmental Panel on Climate Change (IPCC), can generate a petabyte (1 million gigabytes) of data. Weather forecasts involve suites of complex simulations, which are then averaged to assess the probability of different scenarios. These models simulate not only the atmosphere, but the important interactions with the ocean, land and vegetation. Sophisticated models are also used for studying tectonic continental shifts, to understand the geology and climate of previous epochs, thereby informing our understanding of prehistoric life. And similar models are used to simulate hydrological reservoirs and the melting occurring at the base of major glaciers. Computation is so central to the geosciences that it is impossible to imagine the study without it.

The computational approaches relevant for geoscience can be grouped in two classes: simulation and analysis. Geoscientific computation demands advance programming techniques and optimized simulations, to ensure the fast calculations. Changes in the global ocean circulation can take tens of thousands of years, demanding the most rapid simulations possible. High performance computing approaches, for example using graphical processing units (GPUs), are now being applied to climate models, greatly increasing performance. The large amount of data generated by geophysical simulations is also a challenge and is well-suited for big data techniques. Machine learning is beginning to be used in weather forecasting and in climate simulations. This has led to the identification of weather patterns missed by researchers and to the identification of extreme events like cyclones and “atmospheric rivers”, on par with that of human analysts. Computational geoscience is an exciting and developing field, and one which will make major inroads to the earth sciences in the future.

Machine learning in education research. Quantitative education research has historically been done at the micro-scale (classrooms) and the macro-scale (K-12, baccalaureate degree programs, etc.). Micro-scale research has been done using traditional correlational statistics with data gathered from surveys, conceptual tests, classroom observations, etc. With the advent of the *digital classroom* student behavior can now be examined in fine grain. Students access of online homework platforms, video lectures, and interactions with peers via online course forums has created new data sources for education researchers. New technologies such as computer textual analysis can pick apart student conceptual understanding of hard concepts in science and mathematics. Intelligent tutors can provide real time feedback to students as they solve problems. At the macro-scale students’ career decisions within their programs can be modeled. What courses they choose to take, who they choose to take courses from, and their comments on said courses, form new data sets which can be used to predict student decisions and provide timely feedback to students and faculty advisers. Ultimately these data sets can form a high dimensional picture of student learning painted by machine learning.

Appendix D: Outline of degree programs and courses

This appendix summarizes the set of degree programs and courses that can/should be administered by the new department. The range of offerings gives students the opportunity to engage with computational science at a variety of levels, from single courses to graduate programs. Market research and feedback from employers indicate that engaging with one or more of the proposed programs will substantially enhance the student’s career prospects. The new classes will move to the new department once the department opens ist doors.

Degree programs. The MNFak offers from fall 2018 two new programs at the Master of Science level in Computational Science and Data Science. These programs are

1. Computational Science, start fall 2018
2. Data Science, start fall 2018

3. Develop similar Master of Science programs tailored to other colleges at UiO, including the Humanities, Law, the Socials Sciences, Medicine and Education by fall 2020
4. Develop an all university PhD program in Computational Science and Data Science by fall 2020
5. Based on these programs and the gained experiences we plan to develop a Master of Science program in Computational Science and Data Science tailored to the needs of the private and the public sectors. This will allow students residing outside UiO to develop their knowledge about Computational Science and Data Science by fall 2021
6. Develop a PhD program in Computational Science and Data Science tailored to the needs of the public and the private sectors (so-called nærings PhD in Norwegian)
7. Develop a bachelor program in Computational Science and Data Science by 2021

The Master of Science and PhD programs that will target students from outside UiO (from partner companies, public and private sectors) will be developed in close collaboration with external stake holders.

Courses. There are several existing and planned courses which could be offered by the new department. These are

1. FYS-STK4155 Applied Data Analysis and Machine Learning (first time fall 2018)
2. IN4230 High-Performance Computing (first time spring 2019)
3. MAT4110 Computational Mathematics
4. FYS4150 Computational Physics
5. New courses on advanced data analysis and machine learning including for example
   - Supervised and unsupervised machine learning
   - Data analysis and machine learning tailored to the Humanities
   - Data analysis and machine learning tailored to the Social Sciences
   - Data analysis and machine learning applied to Education programs
   - Data analysis and machine learning applied to Law
6. Multi-particle methods for the Physical Sciences and Life Science
7. Courses on quantum computing and quantum information theory

8. Courses on computations in economy
9. Courses on software carpentry and data carpentry
10. ....

Many of these courses, if properly modularized, can be offered as intensive training courses and programs. In particular, such courses will be attractive for both the private and public sectors. The following courses could be offered

1. Introductory Scientific Python
2. Advanced Scientific Python
3. Data Science and visualization
4. Applied numerical mathematics
5. Computational finance
6. Big data graph analysis
7. Supervised machine learning with scikit-learn and TensorFlow
8. Unsupervised machine learning with scikit-learn
9. Data-driven entrepreneurship
10. Courses tailored to the needs of specific companies
11. and more specialized modules

Appendix E: Summary of Timeline

1. Establish a working group by April 1 2018. The working group will be tasked with evaluating various scenarios for strengthening Computational Science and Data Science at UiO. The report will be finalized during Fall 2018.
2. Start establish from spring 2019 a department (or possible center) called **Department of Computational and Data Sciences**, with inauguration by end of 2020/begin 2021.
3. New Master of Science Program on Computational Science starts fall 2018
4. New Master of Science Program on Data Science starts fall 2018
5. Establish a cross-college PhD program in Computational and Data Sciences, start fall 2020. This PhD program will be a collaboration between the Natural Sciences, Humanities, Social Sciences, Medicine and Education.

6. Develop a corresponding cross-college MSc program in Computational Science and Data Science by fall 2020.

7. An undergraduate program in Computational and Data Sciences tailored to various disciplines by fall 2020

8. Develop courses and course modules in Computational Science and Data Science for the private and the public sectors by fall 2019.

9. Develop a Master of Science program and a PhD program in Computational Science and Data Science tailored to the needs of the private and the public sectors, allowing for students residing outside UiO to develop their knowledge about Computational Science and Data Science by fall 2021.

10. Submit an application called **Computing Across the Disciplines** for a Marie Curie training network by spring 2019, 15 PhD positions

Appendix F: Examples of Centers and Departments other places

In Norway it is only UiO which offers a Master of Science program on Computational Science and Data Science. All other universities have only Master of Science programs on Computer Science. The University of Bergen has a Master of Science program on Applied Mathematics while UMB has only a Master of Science on Bioinformatics and Data analysis. These are limited and more focused programs. Nationally, UiO is the only university which offers broad programs in Computational Science and Data Science. The goal in Oslo is to establish a department which covers both Computational Science and Data Science across colleges and disciplines. The department will be responsible for these educational programs and oversee that a coherent and modern selection of courses is offered and developed. The courses should reflect the needs of society at large as well as the specific research projects. This will give UiO a unique position in Norway.

Out of 95 universities polled in the USA, there are less than 15 which have a department on Scientific Computing and more than 50 that have a center on Scientific Computing. Between 20 to 30 of these offer a bachelor, Master of Science or PhD program. On Data Science there are approximately 30 departments and 40 centers. Almost 50 of these universities offer a Masters degree in Data Science and close to 40 a PhD in Data Science. An excellent example of a department which includes computational science and data science is the newly established department at Michigan State University.

For the department of Michigan State University, the process which led to the establishment of the new department started fall 2013 and the new department opened its doors in fall 2015. It counts now 31 faculty of which 24 of them have shared positions with other departments. It offers a series of courses at all levels, minors and majors in Computational Science as well as its own graduate program. The department offers also a dual PhD with other departments. This option has been particularly popular with Physics students.

The new hires cover most STEM fields and the department has been central in starting new cross-disciplinary research activities. There are strong activities in life science and bioinformatics as well as in statistics, mathematics, physics, geoscience and engineering. This department can serve as a role model for the development of a similar department at UiO.

Other departments with similar scope and programs in Northern America are (the list is not exhaustive)

1. School of Computational Science and Engineering at Georgia Institute of Technology
2. Computational Science and Engineering at University of California Santa Barbara
3. Computational Science and Engineering at North Carolina Agricultural and Tecnological State University
4. Computational Science and Engineering at University of Illinois Urbana-Champaign
5. Department of Scientific Computing at Florida State University
6. New York University

Most of the other university in Northern America have a typical department of Computer Science. Programs in Computational Science and Data Science are frequently offered by the department of Mathematics and/or the department of Computer Science.

At the time of writing, no such poll has been made for European universities. From the list over Masters programs, the countries with the largest focus on these topics are Germany (SimTech in Stuttgart is a good example), Sweden and Switzerland. Examples of interest in Europe are the

- London School of Economics
- Imperial College and its Quantitive Sciences Research Institute
- Swiss Institute of Computational Science

while in Austria we have the

- Vienna Graduate School in Computational Science

The Society for Industrial and Applied Mathematics (SIAM) keeps track of graduate programs in computational Science. The list is most likely not complete.

In addition to the traction seen within data driven discoveries, Quantum Information Science (QIS) is also gaining considerable momentum presently. This represents a truly cross-disciplinary activity that cannot be placed within one single department. Though the disruptive potential of QIS has been known for over 20 years, it has been in a nascent state with a number of academic, industrial and government groups striving to understand the basics physics and to build and control many-qubit systems. There has been steady progress to a tipping point where the realization of practical QIS systems is imminent; for example the leading group in the field (Google Quantum AI) recently argued that small-scale commercialization of quantum computing devices is expected within 5 years; moreover quantum chemistry may be a “killer app” for small quantum computing systems; and prototype demonstrations are already emerging. IBM is providing a 20 QUBIT system for public use, and they expect to deliver a 50 QUBIT system in the near future.

Strategic partnerships are developing between universities, large corporations, startups, as well as federal and private funding agencies in the USA. Some of the major industrial and government investors are Google, IBM and Microsoft. In the USA both the Department of Energy and the National Science Foundation are developing QIS programs with several new initiatives.