Computing Across the Disciplines (CAD); a new Center/Department at the University of Oslo

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A proposal to the board of the Mat-Nat Fakultetet of the University of Oslo;
Establish a center by fall 2018 and as a new department by fall 2021

Executive Summary

- Position UiO as a leader in computational science 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).
- 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.
- 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!
- Educate the next generation of school teachers and university teachers, with a strong focus on digital competences.

This proposal seeks to transform Michigan State University into the world leader in scientific discovery through large-scale computation. The Colleges of Natural Science and Engineering propose: (1) a new Department of Computational Mathematics, Science and Engineering (CMSE) that is jointly administered by the College of Natural Science and the College of Engineering, to facilitate interdisciplinary science; (2) the injection of 25-30 new faculty lines focusing on the science of computational modeling and data science; and, (3) the foundation

for joint cutting-edge graduate and undergraduate programs. This effort will open doors to new scientific challenges, will enable MSU to compete for Center-level funding opportunities in computation-related areas that are currently beyond our reach, and will facilitate the training of scientists and engineers to be an effective 21st century workforce. The metrics for success are as follows. Within 5 years, we will have hired the 25-30 worldleading research intensive 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 CMSE to develop large-scale funding. Furthermore, we will have successfully implemented a graduate program (including a graduate certificate, and CMSE and dual PhD and MS programs) and an undergraduate minor. These programs will establish student interest and demonstrate enrollment trends. Finally, this department will facilitate the growth of the university by participating in cross-cutting efforts such as the upcoming quantitative biology initiative. Within 10 years, the initiative will have secured Center-level funding (such as a DOD MURI center, a DOE SciDAC center, an NSF Science and Technology Center, or similar center initiatives coming from NIH or other federal agencies). We will have fully developed our undergraduate curriculum with the addition of Bachelor's programs in computational modeling and data science, and will have strong enrollment numbers in both our minor and B.S. programs - targeting on the order of 400+ minors and 200+ majors. At the graduate level, we will have implemented a professional Master's degree (including an online Master's), and our PhD program will have 75-100 graduate students. CMSE is 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. The CMSE paradigm shift recognizes computation as a new discipline rather than decomposed into isolated sub-disciplines, enabling application-driven computational modeling ("pull"), while also exposing disciplinary computationalists to advanced tools and techniques ("push"), 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 Computational Science and Data Science?

Modern problems in science and engineering bridge a vast range of temporal and spatial scales and include a wide variety of physical processes. 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 insight requires a deep understanding of approximation theory, high performance computing, and domain specific knowledge of the area one is modeling. Our national laboratories 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 (for example, Los Alamos National Laboratory's Computer, Computational, and Statistical Sciences Division3). This collaborative arrangement between algorithmic scientists and disciplinary scientists in the STEM 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, including renewable energy, clean water, and the role of DNA in predicting and maintaining human health. Furthermore, this department would strive to use computing as a critical tool to explore fundamental scientific questions in subjects as diverse as nuclear physics and evolutionary biology. 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, and attracting world-leading talent in this area is greatly facilitated by the introduction of the nurturing environment of CMSE to serve as their tenure home4. Furthermore, the development of the Department of Computational Mathematics, Science, and Engineering will catapult MSU into the position of being a world leader in this critical new field, and will open doors to new scientific challenges as well as new Center-level funding opportunities, such as the DoE SciDAC and NSF OCI SI2 programs (as well as similar programs out of NIH). To jump-start this new department at the 'triple point' of mathematics, computer science and 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. In addition, we wish to recruit scientists - having joint appointments with other units at MSU - whose expertise is 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. Co-location and research and curriculum ties enable CMSE to break down historical disciplinary boundaries, and become the synergistic leading-edge center of computational activities on campus. Furthermore, co-locating these scientists will enhance the development of new computational algorithms to address pressing scientific 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 MSU, bringing researchers in computational and data sciences together with domain experts in energy, clean water, neuroscience, digital evolution, accelerators, logistics, data analytics, and more.

- By 2020, it is expected that one of every two jobs in the STEM fields will be in computing (Association for Computing Machinery, 2013)
- Computation is an essential and cross-cutting element of all STEM disciplines
- Computational science has developed into a discipline of its own right
- Computations and the understanding of large data sets will play an even larger role in basically all disciplines of STEM fields, Medicine, the Social Sciences, the Humanities and education
- Students at both undergraduate and graduate level are unprepared to use computational modeling, data science, and high performance computing – skills valued by a very broad range of employers.
- 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.

Strengths, Possibilities and Synergies.

- Several Centers of excellence in research where Computational Science plays a major role
- 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 fiels who do Computational Science
- Computational topics are included in all undergraduate STEM programs, possibility to develop a bachelor program in Computational Science
- Several educational prizes and awards related to computational science
- 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
- Lead in the development of computations in Life Science
- Strong links with SIMULA research lab

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
- Computational biology and life science (includes medicine)
- Computational economics and data science and computing in the social science
- 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, this 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, reducing redundancy in the courses taught and allowing the university of offer a wider range of more specialized advanced courses. Second, we will create a robust set of degree, minor, and certificate programs that are designed to give STEM students a strong introduction to computing that will complement MSU's existing disciplinary training, and which will make them better suited to be a part of the STEM workforce in the 21st century. These programs will include: a B.S. in Computational Modeling; a B.S. in Data Science (including specializations in bioinformatics and mathematical foundations of data science); a M.S. and PhD in Computational and Data Science; and an undergraduate minor and graduate certificate in Computational and Data Science5. 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 MSU population to learn about some aspects of computational and data science through the minor, graduate certificate, or by taking individual courses. 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 in the sciences and engineering throughout the MSU campus. We

note that a final benefit of these educational efforts is that MSU 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.

Structure and Justification for Planned Organization

We envision that CMSE will be a truly interdisciplinary unit that strives to focus on algorithmic science and its applications to a range of critical research topics. CMSE will consist of 25-30 faculty, comprising generalists and disciplinary scientists. The generalists develop crossdisciplinary 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 CMSE unique. The joint College of Natural Science and College of Engineering committee that developed this proposal seeks the creation of a joint, inter-college department as the ideal solution. This structure, where tenure lines would be housed, 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 here at Michigan State University 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 science and engineering. By placing the tenure 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 STEM disciplines. Second, the new department will break down traditional barriers between departments in the Colleges of Natural Sciences and Engineering, as the common theme of the new department is the science of algorithms and their application to problems in science and engineering, providing a key place for critical interactions between these 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 MSU 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. In the case of joint appointments, the department with the majority appointment will lead on issues of reappointment, promotion, and tenure. For all faculty appointed in the new unit, either fully or partially, a key consideration in reappointment, promotion, and tenure will include the

development of algorithms and computational codes and libraries that contribute broadly to the advancement of research. A potentially major issue with the proposed format is that a great deal of teaching capacity will be required to launch the new undergraduate and graduate programs. Consolidation of existing classes on campus will free up some teaching slots; however, to ensure success we propose teaching slots be assigned to the new unit based on percentage appointment within the new department. For example, if the faculty has 50% appointment within this new unit and is assigned a 1-1 teaching load, one of the courses they teach each academic year will be assigned by this new department. A key point in making this new unit work is the creation of a robust community of scholars. To that end, it is key that the new faculty and graduate students in this department be co-located within the same space. We propose the creation of a common space that can hold a substantial number of people, including 25 to 30 faculty, up to 10 visitors, up to 6 support staff, and approximately 100 postdocs and graduate students. This space needs state-of-the-art computing classrooms, conference rooms configured for video conferencing, and resources for teaching in flipped and virtual classroom settings. Currently, this is under discussion between CNS and EGR, and several locations are under consideration. Another key point in the success of such a department is the influx of new ideas and people. In lieu of teaching specialists, we propose recurring funds to support 50% teaching activities of interdisciplinary postdoctoral researchers (balance supported by fellowships and research grants), as well as funds for a long-term visitor/recruitment program that would aim to have at least two long term faculty-level visitors in residence at any given time in order to inject new ideas. Combined, this will help to keep the unit current in terms of the latest computational methods and scientific problems, and will assist in the attraction of top talent to MSU.

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. This will be realized by the securing of Center-level funding (as well as many single- or few-PI grants), as well as the creation of a coherent academic program with large undergraduate and graduate enrollments. We anticipate that each PI will bring in between $200K-$400K per year in grants, on average. This will fully fund between 3-6 graduate students per PI, plus travel and other associated expenses. In order to ensure the success of these efforts, the proposed department must be financially sustainable. Continued 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. There are a variety of mechanisms to provide this funding, including:

- The development of an online Master's degree in data science and informatics.
- The development of an online Master's degree in applied computation.

- Teaching assistantships for high-quality graduate students who need support. These positions will be TAs for introductory undergraduate and graduate computing courses.
- The program will aggressively pursue endowments for fellowships, visitors, and faculty chairs.

Taken in combination, these sources of continued funding will be critical to the sustained success of this new department.

The Center/Department.

- Administratively located under the Mat-Nat college
- Composed of 25-30 full time equivalent positions, including some current UiO faculty and when it becomes a department a larger number of new hires.
- Most of these faculty will have joint appointments with other units and/or departments at the University of Oslo and SIMULA research laboratory. As an example, one can have a 70% appointment in Mathematics and 30% at the new department.
- Faculty will focus on computational science, data science and large-scale and high-performance computation
- Faculty will be incentivized to engage in cross disciplinary and cross-department/college research collaborations
- Nurturing environment to attract these faculty and pursue large and interdisciplinary grants
- Close ties to SIMULA research laboratory and the HPC center at USIT

Benefits.

- Recruitment of new faculty who are incentivized to collaborate across the university both in terms of research and education.
- Opportunities for existing UiO faculty to expand their computation-related capabilities, and to train students to use computational techniques.
- Broad and deep educational opportunities for both undergraduate and graduate students across the university.

Research opportunities.

- Data driven discovery and data-driven modeling where machine learning plays a central role
- Research challenges that require computation-oriented multidisciplinary and interdisciplinary approaches.
- Research problems that require "bleeding edge" (e.g., multi-petaflop/petabyte) computational approaches to interpret experimental data and complex data.
- Computational and data science research and education scattered across many departments. New department can strengthen computational science.
- Develop research programs on Quantum Computing, the future of computing. The Wallenberg foundation in Sweden and Chalmers University of technology have funded a project on developing quantum computing technologies with SEK 1 billion. The aim is to position Sweden in a top global top position in quantum technology.
- Center-level funding opportunities (e.g., SFF, Marie Curie etc etc).
- Simulations of complex quantum mechanical systems using novel algorithms, with applications spanning from quantumchromodynamics on the lattice and subatomic physics, via materials to the equation of state of stars.
- Exploring algorithms from quantum computing in order to solve complicated quantum mechanical problems
- Study complex materials or the DNA using large-scale molecular dynamics simulations
- Using machine learning to solve complicated problems, from neuroscience (our brain), physiology to complicated materials
- Using machine learning to develop new tools for learning
- Bioinformatics, Computational Biology and Life science
- Computational economy and computing in the Social Sciences
- Data-driven discovery and modeling in the Humanities

Possible steering committee (2018)

1. Institute for theoretical Astrophysics and Rosseland Center for Solar Physics: Mats Carlsson and Viggo Hansteen
2. Bioscience: Tom Andersen and Lex Nederbragt

3. Chemistry and Hylleraas Center for Quantum Molecular Sciences: Michele Cascella, Thomas Bondo Pedersen, Trygve Helgaker and Simen Kvaal
4. Geoscience: John Burkhart, Joe Lacasce and Thomas Vikhamar Schuler
5. IFI Bioinformatics: Torbjørn Rognes
6. IFI Imaging and Biomedical Computing (coupling to Simula): Andreas Austeng, Xing Cai, Joakim Sundnes and Simon Funke
7. Math and Mechanics: Karsten Trulsen and Kent-Andre Mardal, Andreas Carlsson
8. Math and Computational Finance, Statistics and Risk Analysis: Arne Bang Huseby and Geir Olve Storvik
9. Math and Cmputational Mathematics: Geir Dahl, Ragnar Winther, Knut Mørken, Martin Reimers, Michael Floater
10. Physics and Center of Computing in Science Education: Morten Hjorth-Jensen and Anders Malthe-Sørenssen
11. Medicine: need people
12. UV: Anders Kluge
13. Social Sciences: Kjetil Storsletten and Halvor Mehlum
14. Humanities: need people

Timeline.

1. Establish a center called **Center for Computing across Disciplines** by Fall 2018 and co-locate with the new Center for Computing in Science Education
2. Establish a department called **Department of Computational and Data Sciences** by Fall 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. Extend these Masters progrms to become cross-college programs
6. 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.
7. Develop a Bachelor program in Computational Science and Data Science? Need to strike a balance between existing programs and possible new **honors program**.

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

9. Submit an application called **Computing Across the Disciplines** to the Norwegian Research council by Spring 2019, 10 PhD and 10 PD positions

10. Prepare first draft for an SFF application by spring 2020

Centers and Departments at other universities

In Norway it is only UiO which offers a Masters program on Computational Science and Data Science. Al other universities have only Master programs on Computer Science. The University of Bergen has a Masters program on Applied Mathematics while UMB has only a Masters 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.

Norway	University	Comp Science and Data dept	Bachelor program	Master program
	UiO	No	No	Yes
	NTNU	No	No	No
	UiT	No	No	No
	UiB	No	No	No
	UMB	No	No	Yes (Bioinf+stat datanalys

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.

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, Sweden and Switzerland.

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.

Educational programs at other universities

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

Research programs