Computational Mathematics, Science and Engineering (CMSE): Establishing an Academic Department Dedicated to Scientific Computation as a Discipline

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1. ABSTRACT

The Computational Mathematics, Science and Engineering (CMSE) department is one of the newest units at Michigan State University (MSU). Founded in 2015, CMSE recognizes computation as the "triple junction" of algorithm development and analysis, high performance computing, and applications to scientific and engineering modeling and data science (as illustrated in Figure 1). This approach is designed to engage with computation as a new integrated discipline, rather than a series of decentralized, isolated sub-specialties. In the four years since its inception, the department has grown and flourished; however, the pathway was sometimes arduous. This paper shares lessons learned during the department's development and the initiatives it has taken on to support computational research and education across the university. By sharing these lessons, we hope to encourage and support the establishment of similar departments at other universities and grow this integrated approach to scientific computation as a discipline.

Keywords

Computational science; academic department administration.

2. INTRODUCTION

Establishing an entirely new department is no trivial task. One immediate hurdle is finances: the traditional university funding model would require that existing departments give up a portion of their budget in order to free up funds to create a new unit. At Michigan State University (MSU), the concept of Computational Mathematics, Science and Engineering (CMSE) was discussed at length and many faculty and administrators could see the potential for positive impact - but no one wanted to lose their existing funding. As part of these discussions, many alternatives to creating a new department were considered. For example, CMSE could have developed as a new focus area within an existing department (such as Computer Science & Engineering) or could have been the central theme for a new cross-disciplinary center or institute within

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Figure 1: Triple Junction of algorithm development and analysis, high performance computing, and applications to scientific and engineering modeling and data science

the University's research unit. These solutions do not provide the same long-term foundation and commitment that results from the formation of a new department, however.

Fortunately, in the early 2010s MSU announced its Global Impact Initiative (GII) [2], which offered new resources to bring more than 100 additional faculty to the university to pursue solutions to "Grand Challenges." One of these grand challenges was the continued advancement of computation in science, and the proposal to create a new CMSE department was an obvious fit for the MSU GII. Almost all faculty in the new department have joint appointments with other units, which created opportunities to leverage the GII funding to simultaneously create CMSE and grow the faculty in programs across campus.

The idea of "jointness" has been ingrained into the culture of CMSE from the beginning. The department is shared between the College of Natural Science and the College of Engineering. Faculty wear multiple "hats," typically in CMSE and in another STEM (science, technology, engineering, math) unit on campus. The department was designed from the start to encourage faculty to speak from two valued perspectives: the common language we are developing in CMSE, and the traditional language of their STEM departments.

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Figure 2: The new department is shared between two colleges and almost all faculty have joint appointments between CMSE and another department.

The CMSE department is home to computational thinkers from many fields and actively fosters discussion and collaboration across disciplines. 10 existing MSU faculty transferred (part of) their appointments into CMSE and the department conducted numerous searches to bring in 25 new, external hires. These faculty members have expertise in a range of science and engineering areas, as illustrated in Figure 2, as well as a variety of experience. Of the 35 faculty members of CMSE in Summer 2019, 22 were Assistant Professors, 3 were Associate Professors, 7 were Full Professors, and 3 were Academic Specialists (faculty not on a tenure track). In Fall 2019, 3 new hires are slated to join the faculty and the plan is to grow CMSE to 50 faculty members over the next few years.



Figure 3: Figure 3: Growth rate of the CMSE community. Measured by tracking faculty, staff, researchers and full-time students within the department email list.

The rapid growth within CMSE (see **Error! Reference source not found.**) has not always been easy. Early on, senior faculty were burdened with abnormally high service requirements, in part because the many junior faculty needed to focus on earning tenure. The joint-appointment standard within CMSE meant that the department had to overcome many bureaucratic hurdles to ensure that tenure processes were aligned for faculty whose appointments spanned multiple colleges and/or departments. The diverse backgrounds of our faculty brought the benefit of different perspectives, but also meant that we had to work hard to establish effective communications across disciplines and research efforts. Several years in, however, the department seems to have hit its stride. While these problems have not gone away entirely, we have strong leaders and effective plans in place to help ensure the continued growth and success of the department and its academic and research programs.

3. UNDERGRADUATE EDUCATION

At MSU, all STEM undergraduates are expected to take some combination of common "gateway" courses (e.g., calculus, chemistry, physics, biology). CMSE has developed two scientific modeling courses: Introduction to Scientific Modeling (CMSE 201) and Tools for Scientific Modeling (CMSE 202). These courses focus on learning to program in the context of solving scientific and engineering problems and contribute to a parallel effort across MSU to add "computational competency" to the "gateway" learning goals for all STEM majors. Ideally, all STEM students will learn basic programming concepts within their first two years at MSU, which will enable instructors in higher level courses to use programming as a tool to more effectively teach other STEM concepts. For example, computational competency is now a requirement for all Physics majors and is a prerequisite in courses such as Linear Algebra (Math/CMSE 314), which uses real world examples and computational methods to teach Linear Algebra

The CMSE 201/202 course use a Flipped Classroom style of teaching that focuses on hands on learning inside of the classroom, with accompanying lectures provided in videos watched outside of class (see Figure 5). This course pedagogy is grounded in learning sciences [1] and is growing rapidly (see Figure 5).

Students who are excited by what they learn in CMSE 201/202 now have the option of earning an undergraduate minor in Computational Modeling and Data Science. This minor is targeted primarily at STEM students but is open to undergraduates from across the university. This minor gives students a solid background in programming and computational science through a 2-3 semester introductory course sequence; additional exposure to a breadth of methods in computational and data science, including a disciplinary-specific computational course; and options for a research experience or project-focused "capstone" course.



Figure 4: Growth of 201/202 Enrollment by year as the CMSE department grows to serve the MSU STEM community

Starting in Fall of 2019, MSU is offering a new undergraduate major in Data Science. This program is a collaboration between multiple departments (CMSE, Statistics, Computer Science), and MSU is working with other institutions to develop a common set of competencies for data science programs [3], We are very cognizant of the current hype surrounding data science and machine learning, and the explosion of "data science" programs across higher education. Unfortunately, the term data science is not well defined and there is not yet a standard understanding of the content of a "data science" degree. As part of its overarching mission to help establish data science as a discipline, CMSE is working across disciplines within MSU – and across institutions more broadly – to help define the disciplinary standards for data science programs.

4. GRADUATE EDUCATION

In 2016, CMSE launched three program options for graduate students: the Master's of Science, the Doctor of Philosophy, and a dual-major PhD program that allows students to combine CMSE with another doctoral major at MSU. These graduate programs are designed to help students develop broad skills for solving problems through computational modeling, data exploration, and high-performance computing techniques. Our graduate alumni will have acquired a broad range of computational skills, as well as substantial expertise in solving mathematical and statistical problems using scientific methods.

In Fall 2019, CMSE included 43 PhD students; 2 dual enrollment BS+MS students; approximately 25 dual-major PhD students; and 15 postdoctoral researchers. The CMSE graduate curriculum features a core set of courses in mathematical, numerical and computational methods: numerical linear algebra; numerical differential equations; parallel computing; and the mathematical foundations of data science. With this foundation, students may choose additional coursework that is tailored to their research interests; common examples include graduate courses in physics, applied mathematics, engineering and/or computer science. In addition to completing coursework, PhD students must pass qualifying exams in the four areas covered by the core curriculum and must write and defend a dissertation research plan for their comprehensive exam. The PhD is awarded upon completion and successful defense of their research dissertation.

The dual-major PhD option is administered by the MSU Graduate School and is open to all doctoral students at the University [4]. Students matriculate in one primary major, and then work with advisors to develop a cross-disciplinary program of coursework and research spanning an additional major area of study. Individual program plans are developed for each student pursuing a dualmajor PhD and are generally put into place within the first 12-18 months of graduate studies. Upon successful completion of the individualized program, students earn a single Doctor of Philosophy diploma that reflects both majors.

CMSE has established a dual-major PhD pathway that allows students to pursue a substantial, novel, computationally-focused research program in consultation with at least one advisor (committee member) in CMSE; other advisors (committee members) may be drawn from any appropriate unit on campus [5]. CMSE already has the most dual-major PhD students of any department in the College of Engineering (the department's administrative home), and we anticipate that this interdisciplinary PhD option will be an advantage in recruiting new graduate students with novel research paths. For example, a typical dualmajor PhD student in CMSE might be developing algorithms that are more computationally in-depth than is typical in their home discipline. By creating a dual-major PhD program, these students can craft a set of course and research requirements specific to their area of interest and gain access to the faculty and university resources to support their success.

Beyond the foundational graduate courses, the CMSE curriculum is designed to be nimble and allow faculty and students to explore new topics and research challenges as they arise. For example, in Fall 2019, the department offered nine special-topics courses on the following topics:

- Optimization
- Mathematical reasoning
- Foundations of computational science and engineering
- Applied machine learning
- Programming foundations for bioinformatics
- Statistical analysis and visualization of biological data
- Gaps and errors in statistical data analysis
- Applied linear algebra
- Applied calculus for bioinformatics

To illustrate the utility of this special-topics model, consider a specific example from Fall 2018, when several faculty jointly offered a course entitled "Algorithms for next-generation architectures." Students explored several different types of generalpurpose graphical processing units (GPGPUs) and fieldprogrammable gate arrays (FPGAs) and the software technologies required to use this hardware efficiently. The course encouraged students to think carefully about how to choose and develop algorithms that efficiently use a specific type of hardware to solve their problems. This course, like most graduate and undergraduate courses in CMSE, was taught in a "flipped" manner: students did substantial reading and other preparation prior to class, then during class they discussed these assignments, solved mathematical problems and proofs, wrote software, and analyzed data (see Figure 5). This teaching method has been shown to be very effective in a range of undergraduate STEM courses and has also been well received in our graduate courses.



Figure 5: Example of flipped classroom, where students use classroom time to solve real world problems in groups.

5. COMPUTATIONAL EDUCATION

In addition to establishing traditional undergraduate and graduate programs, CMSE seeks to support the development of computational competency more broadly. For example, the department has developed two graduate certificate programs, one in Computational Modeling and another in High Performance Computing [6]. These stand-alone certificates are earned by

completing at least three courses (9 credits) from a list of approved options. Working professionals may enroll as lifelong learners (non-degree students) and pursue a certificate program to enhance their skills, or graduate students in other MSU programs may choose to complete a CMSE certificate in addition to their Master's or Doctoral program requirements. In the longer term, we hope to create a pathway that would allow non-traditional students to earn a Master's degree by completing several standalone certificates over time along with a culminating capstone experience. This could provide additional flexibility for working professionals who are not interested or able to pursue a full-time graduate program.

CMSE has also created a Bioinformatics Program to offer short, modular, introductory courses focusing on the development of basic skills in computation and bioinformatics. This program addresses the needs of MSU graduate students in biological sciences, who often seek additional training in how to work with the very large data sets now common in the life sciences. These short courses are designed to help students gain skills that can be immediately applied to their coursework and research, as well as helping to build computational competency and skills that can be leveraged if the students wish to pursue more advanced CMSE coursework.

6. CONCLUDING DISCUSSION

CMSE is uniquely positioned at the "triple junction" of algorithm development and analysis, high performance computing, and applications to scientific and engineering modeling and data science. In the four years since its inception the department has grown and flourished, establishing both traditional degree programs and non-traditional options to build computational competency in learners from across STEM. As the department continues to mature, we hope to support the formation of similar units at other institutions and to help shape the emerging discipline of scientific computation.

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8. REFERENCES

[1] Brian Danielak, Brian O'Shea, and Dirk Colbry. 2016. Using Principles from the Learning Sciences to Design a Data-Driven Introduction to Computational Modeling. In *Workshop on Teaching Computational Science (WTCS)*.

- [2] Global Impact Initiative | Research at Michigan State University. https://research.msu.edu/global-impact/
- [3] 2019 Data Science Leadership Summit, Nov 7-9, Santa Fe, https://sites.google.com/msdse.org/datascienceleadership201 9/home
- [4] Interdisciplinary Programs | MSU Graduate School. https://grad.msu.edu/interdisciplinaryprograms
- [5] Dual PhD in Computational Mathematics, Science and Engineering. https://cmse.msu.edu/academics/graduateprogram/dual-phd-in-cmse/
- [6] Graduate Certificates | Computational Mathematics, Science and Engineering. https://cmse.msu.edu/academics/graduateprogram/grad-certificates/