# **Center for Computational Science and Engineering**

The Center for Computational Science and Engineering (CCSE) was established in 2008 within the School of Engineering as the Center for Computational Engineering (CCE), to support computational engineering research and education at MIT. Over time, CCE's activities in science increased – markedly so in recent years as departments within the School of Science—Mathematics and Earth, Atmospheric, and Planetary Sciences decided to join the center's computational science and engineering PhD program. At the same time, core subjects for the center's master and PhD programs have become listed across various departments spanning the Schools of Science and Engineering, and are being co-taught by teams of faculty from both schools. Concurrently, as plans for the MIT Stephen A. Schwarzman College of Computing began taking shape, our center joined the conversation, and by fall 2019 was slated to become one of its inaugural core academic units. A number of factors-our significantly increased engagement with science, the impending move out of the School of Engineering, the fact that "Computational Science and Engineering" (CSE) had become the nationally recognized name of the field as well as the name of the center's doctoral program—led to a strong argument for the center to be renamed the Center for Computational Science and Engineering. This renaming was approved by the Institute effective January 1, 2020, in conjunction with CCSE's move to the Schwarzman College of Computing. Looking ahead, CCSE is expected to "play a substantial role in the numerical, simulation and data science curriculum and classes in the Common Ground, possibly eventually including minors or additional degrees."

Following on the success of an expanded annual symposium in 2019, the 2020 CCSE Annual Symposium was scheduled to take place in conjunction with our admitted student visit day on March 19, 2020, at the Boston Marriott Cambridge. On the agenda were talks from three MIT CCSE-affiliated faculty members (Bilge Yildiz, professor of nuclear science and engineering and professor of materials science and engineering; Raffaele Ferrari, Cecil and Ida Green Professor of Oceanography; and Wim van Rees, assistant professor of mechanical engineering) as well as a keynote by Nick Trefethen, professor of numerical analysis at the University of Oxford. An announcement of the MIT CCSE MathWorks Prize winners, a student poster session, and a reception would have completed the schedule of events. Due to the COVID-19 pandemic and resulting Institute policies, however, this event and the admitted student visit day were cancelled in early March. A series of virtual information sessions were offered via Zoom to the admitted students, and we made plans to reschedule the symposium at a future date when it is safe to do so.

Replacing the in-person announcement and celebration, the MathWorks Prizes for Outstanding Doctoral and Masters Research were announced via email to the CCSE community and posted on the CCSE website and Facebook page. The prize for Outstanding Doctoral Research, Computational Science and Engineering Program was awarded to Chinmay Kulkarni. Chinmay is a CSE graduate student in MIT's Department of Mechanical Engineering working with Professor Pierre Lermusiaux. The prize for Outstanding Masters Research, Computation for Design and Optimization Program was awarded to Tony Tohme, who works with Professor Kamal Youcef-Toumi of the Department of Mechanical Engineering.

## **Professional Development Programs**

Over the past year, CCSE faculty have worked with MIT Open Learning and MIT xPRO to develop a new online educational program aimed at industry professionals. The program is called "Machine Learning, Modeling, and Simulation: Engineering Problem-Solving in the Age of AI." It aims to bridge computational science and engineering principles—and the science/engineering applications where CSE has had greatest impact-with recent methodological advances in machine learning and artificial intelligence. It consists of two online courses, the first titled "Machine Learning, Modeling, and Simulation Principles" and the second "Applying Machine Learning to Engineering and Science." Professor Youssef Marzouk serves as faculty director for the program, and the primary instructor of the first course. The second course comprises modules taught by Marzouk and eight other CCSE faculty instructors: George Barbastathis (Mechanical Engineering), Richard Braatz (Chemical Engineering), Markus Buehler (Civil and Environmental Engineering), Laurent Demanet (Mathematics), Heather Kulik (Chemical Engineering), Themis Sapsis (Mechanical Engineering), Justin Solomon (Electrical Engineering and Computer Science), and John Williams (Civil and Environmental Engineering). Development of exercises and other materials in the first course was aided by four CSE PhD graduate students who were employed by MIT xPRO: Ricardo Baptista, Michael Brennan, Elizabeth Qian, and Benjamin Zhang. The first run of the program, from April to June 2020, drew roughly 130 remote learners. CCSE plans to support MIT xPRO as they improve the course and offer it three times a year.

## **Graduate Education**

CCSE offers two educational programs, the interdisciplinary Master of Science Program in Computation for Design and Optimization (CDO) and the Doctoral Program in Computational Science and Engineering (CSE).

## **Computation for Design and Optimization**

Computation for Design and Optimization enrollment at the start of AY2020 was 18 students, nine of whom were entering first-year students. Two CDO students graduated on the September 2019 degree list, one graduated on the February 2020 list, and four graduated in May 2020, increasing the total number of CDO alumni to 180 as of May 2020.

CDO conducted its 16th admissions cycle this past winter and spring. Serving on the admissions committee with Nicolas Hadjiconstantinou and Youssef Marzouk were Rafael Gomez-Bombarelli (Materials Science and Engineering) and Justin Solomon (Electrical Engineering and Computer Science). Out of a total applicant pool of 115, nine were admitted (an 8% admission rate). One student enrolled in February 2020, and five accepted to begin their master of science degree in September 2020 (a yield of 67%). However, because of the pandemic, two of the five have deferred to September 2021. A student who deferred during the previous admission cycle will be joining the 2020 cohort for a total expected enrollment of four new students in September 2020.

During spring 2020, with the support of affiliated faculty, current students, alumni, and Dean Dan Huttenlocher, we submitted a request and received approval from the Committee on Graduate Programs to change the name of CCSE's SM degree program

from "computation for design and optimization" to "computational science and engineering." With this change, the names of the center, the interdisciplinary master's degree program, and the interdepartmental PhD program are finally consistent. The CSE name also better reflects the scope of the education received by our master's students and is better aligned with the terminology being used across industry and academia, both nationally and internationally. This change will be effective for the September 2020 degree list with additional references to CDO (e.g., CDO.THG) phasing out over the course of the next academic year.

#### **Computational Science and Engineering**

We began accepting applications for our doctoral program in Computational Science and Engineering in September 2013. CSE enrollment at the start of AY2020 was 43 students; three were first-year students and an additional seven current doctoral students in affiliated home departments joined over the course of the academic year. Two CSE students graduated on the September 2019 degree list, six graduated on the February 2020 list, and four graduated in May 2020, bringing the number of CSE alumni to 47.

CSE conducted its seventh admissions cycle this past winter and spring, receiving 133 applications. Hadjiconstantinou and Marzouk served as CCSE reviewers, reading all applications and passing the most qualified applicants along to the various home department(s) for review. Of the 133 applicants, 15 were admitted (an 11% admission rate); five students accepted and plan to begin their degree work in September 2020, with an additional student deferring enrollment to February 2021.

#### **Distinguished Seminar Series in Computational Science and Engineering**

This Institute-wide seminar series hosted by CCSE draws a broad audience from mathematics, science, and engineering but focuses on innovative methods and applications of computation. The AY2020 seminar series included the following invited speakers and topics:

- Michael Mahoney, International Computer Science Institute and Department of Statistics, University of California–Berkeley: "Making the Deep Learning Revolution Practical through Second Order Methods"
- Daniel Simpson, Assistant Professor of Statistical Sciences, University of Toronto: "Sometimes All We Have Left Are Pictures and Fear"
- Na Li, Thomas D. Cabot Associate Professor in Electrical Engineering and Applied Mathematics, School of Engineering and Applied Sciences, Harvard University: "Online Learning and Multiagent Reinforcement Learning in Optimal Control for Linear Time-Invariant Systems"
- Eric Darve, Professor of Mechanical Engineering and Computational Mathematics, Stanford University: "Deep Neural Networks for Inverse Modeling"
- Pierre Gentine, Associate Professor, Earth and Environmental Engineering, Earth Institute, Data Science Institute, Columbia University: "Hybrid Modeling: Best of Both Worlds?"

• Boris Kozinsky, Associate Professor, Computational Materials Science, School of Engineering and Applied Sciences, Harvard University: "Insights from Ab-Initio and Ex-Machina Atomistic Computations into Dynamics of Electrons, Phonons and Ions"

The following spring 2020 seminars were cancelled due to COVID-19:

- Nilima Nigam, Professor of Mathematics, Simon Fraser University
- Andrew Stuart, Bren Professor of Computing and Mathematical Sciences, California Institute of Technology
- Nils Thuerey, Associate Professor of Computer Science, Technical University of Munich
- Lin Lin, Associate Professor of Mathematics, University of California–Berkeley

Nicolas Hadjiconstantinou Co-director Professor of Mechanical Engineering

Youssef Marzouk Co-director Professor of Aeronautics and Astronautics