

Center for Computational Science and Engineering

Established in 2008 and incorporated into the Schwarzman College of Computing as one of its core academic units in January 2020, the [Center for Computational Science and Engineering \(CCSE\)](#) is an interdisciplinary research and education center focused on innovative methods and applications of computation. CCSE involves faculty, researchers, and students from MIT's Schools of Engineering, Science, Architecture and Planning, and Management, as well as other units of the Schwarzman College of Computing. Our educational programs seek to train future generations of computational scientists and engineers to both develop and use sophisticated computational methods for a wide variety of applications.

Although CCSE's activities throughout the 2020–2021 academic year were primarily virtual, we were still able to engage our community and offer a widely attended Distinguished Seminar Series and annual symposium. The 2021 MIT CCSE Symposium took place in a virtual format on March 15, 2021, through a combination of Zoom and Gather platforms. University of Oxford professor Nick Trefethen was the keynote speaker with his talk "From the Faraday cage to lightning Laplace and Helmholtz solvers." Three CCSE-affiliated faculty members also gave talks during the event:

- Raffaele Ferrari, Cecil and Ida Green Professor of Oceanography, "Improving the physics of climate (ocean) models"
- Wim van Rees, assistant professor of mechanical engineering, "Flow simulations for bio-inspired underwater devices"
- Bilge Yildiz, professor of nuclear science and engineering and materials science and engineering, "Electro-chemo-mechanical field effects on electronic properties of functional oxides"

Students from the Computational Science and Engineering (CSE) SM and PhD programs presented their research during the student poster session that followed. Abhinav Gupta, a mechanical engineering student in the CSE PhD program advised by Pierre Lermusiaux—the Nam Pyo Suh Professor of Mechanical Engineering and associate department head for operations—received the best poster award for his contribution "Neural closure models for dynamical systems." A virtual reception followed at the conclusion of the student poster session, during which the winners of the annual CSE MathWorks Research Prizes were announced. The winners were:

- Ricardo Baptista, aeronautics and astronautics–CSE PhD student advised by Youssef Marzouk, professor of aeronautics and astronautics
- Nisha Chandramoorthy, Mechanical Engineering–CSE PhD student advised by Qiqi Wang, associate professor of aeronautics and astronautics

Professional Development Programs

Since mid-2019, CCSE faculty have worked with MIT Open Learning and MIT xPRO to develop "Machine Learning, Modeling, and Simulation: Engineering Problem-Solving in the Age of AI," a new online educational program aimed at industry professionals.

This program aims to bridge computational science and engineering principles—and the science and engineering applications where CSE has had greatest impact—with recent methodological advances in machine learning and artificial intelligence. It consists of two online courses, “Machine Learning, Modeling, and Simulation Principles” and “Applying Machine Learning to Engineering and Science.” 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).

The program launched in April 2020, with the first run (from April to June 2020) drawing roughly 130 remote learners. Subsequent runs of the program drew similarly sized audiences: September–December 2020 (Run 2), February–April 2021 (Run 3), April–June 2021 (Run 4), and September–December 2021 (Run 5, planned). Many of the CCSE faculty involved in the course have continued to support MIT xPRO as they iterate on and improve the course material.

Graduate Education

CCSE offers two graduate educational programs: a doctorate and a master’s degree in computational science and engineering.

Computational Science and Engineering Master of Science

During spring 2020, with the support of affiliated faculty, current students, alumni, and Dean Daniel Huttenlocher, we submitted a request to 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” (CDO) to “computational science and engineering.” The change was effective for the September 2020 degree list, with the two students on the September list receiving the inaugural MIT CSE SM degrees. Shortly afterward, the Registrar’s office officially recoded all former CDO M students as CSE M, solidifying the shift. CCSE staff worked with various Institute offices over the remainder of the fall term to ensure the update was reflected in all other facets of MIT systems and records. The final reference to CDO is the thesis research subject CDO.THG, which will phase out when the final graduate student who enrolled in the subject graduates (due to Registrar policy). Students starting fall 2021 and later will register for CSE.THG.

Enrollment in the SM program at the start of academic year 2021 was 14 students, four of whom were entering first-year students. As previously mentioned, two students graduated on the September 2020 degree list, three on the February 2021 list, and five graduated in June 2021, increasing the total number of SM alumni to 190 as of June 2021.

The SM program conducted its 17th admissions cycle this past winter and spring. Serving on the admissions committee with us—Nicolas Hadjiconstantinou, professor of mechanical engineering, and Marzouk—were Markus Buehler (Civil and Environmental Engineering), Rafael Gomez-Bombarelli (Materials Science and Engineering), Chris Rackauckas (Mathematics), Justin Solomon (Electrical Engineering and Computer Science),

and Wim van Rees (Mechanical Engineering). Out of a total applicant pool of 478, 14 students were admitted, one deferred to September 2022, and nine accepted. An admitted student who had to defer from the previous admission cycle due to the pandemic will be joining this cohort for a total expected enrollment of 10 new students in September 2021.

Computational Science and Engineering PhD

The Computational Science and Engineering PhD program allows students to specialize at the doctoral level in a computation-related field of their choice through focused coursework and a doctoral thesis. In September 2020, MIT's Department of Materials Science and Engineering (DMSE) received Institute approval to join the CSE PhD program in addition to the Departments of Aeronautics and Astronautics; Chemical Engineering; Civil and Environmental Engineering; Earth, Atmospheric and Planetary Sciences; Mathematics; Mechanical Engineering; and Nuclear Science and Engineering as the eighth department to join the multi-departmental doctoral program since its start in 2013. DMSE will award degrees under the thesis field "Computational Materials Science and Engineering" starting in September 2021.

Enrollment in the CSE doctoral program at the start of AY2021 was 58 students, including nine first-year students with an additional eight current doctoral students in affiliated home departments joining over the course of the academic year. Eight CSE students graduated on the September 2020 degree list, four graduated in February 2021, and three graduated in June 2021, bringing the CSE PhD alumni total to 62 as of June 2021.

During the winter and spring of 2020–2021, the CSE PhD program conducted its eighth admissions cycle and received 162 applications. Professors 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 162 applicants, 19 were admitted, 12 of whom accepted and plan to begin their degree work in September 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, and focuses on innovative methods and applications of computation. The 2020–2021 seminar series was conducted remotely via Zoom and included the following invited speakers and topics, captioned recordings of which are available on the CCSE YouTube channel.

- Lin Lin, associate professor of mathematics, University of California, Berkeley, and faculty scientist, Mathematics Group, Berkeley Lab Computational Research Division, "Quantum numerical linear algebra"
- Nils Thuerey, associate professor, Computer Science, Technical University of Munich, "Differentiable physics simulations for deep learning algorithms"
- Tapio Schneider, Theodore Y. Wu Professor of Environmental Science and Engineering, California Institute of Technology, and senior research scientist at NASA's Jet Propulsion Laboratory, "Earth System Modeling 2.0: Toward data-informed climate models with quantified uncertainties"

- Dion G. Vlachos, Department of Chemical and Biomolecular Engineering, Catalysis Center for Energy Innovation, RAPID Manufacturing Institute, Delaware Energy Institute, University of Delaware, “Data science and multiscale modeling for chemical sciences”
- Jacqueline Chen, senior scientist, Combustion Research Facility, Sandia National Laboratories, “Towards DNS of turbulent combustion at the Exascale”
- Aidan Thompson, Center for Computing Research, Sandia National Laboratories, “High-fidelity large-scale atomistic simulations of materials using LAMMPS, SNAP interatomic potentials, and massively parallel computers”
- Georg Stadler, professor of mathematics and computer science, Courant Institute of Mathematical Sciences, New York University, “Estimation of extreme event probabilities in complex systems governed by PDEs”
- Krishna Garikipati, professor, Department of Mechanical Engineering and Department of Mathematics, and director, Michigan Institute for Computational Discovery and Engineering, University of Michigan, “Bayesian neural networks for weak solution of PDEs with uncertainty quantification”

Nicolas Hadjiconstantinou, Co-director
Professor of Mechanical Engineering

Youssef Marzouk, Co-director
Professor of Aeronautics and Astronautics