

# Report to the President, year ended June 30, 2024, 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 MIT [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.

## GRADUATE EDUCATION

During the period of July 2023 - June 2024 CCSE administered two and launched a third graduate program in computational science and engineering (CSE). The two already existing programs are the [master's degree in computational science and engineering](#) (CSE SM) and the [interdisciplinary doctoral program in computational science and engineering](#) (Dept-CSE PhD); the latter is offered jointly with eight participating departments in the Schools of Engineering and Science. After receiving approval in May 2023 to launch the new [standalone doctoral program in computational science & engineering](#) (CSE PhD), considerable time was devoted to preparations for the new program including updated Bulletin listings, advertising and updating our admissions processes, inclusive of transitioning our application from GradApply to Slate to allow a single admission portal to be used for applications to both CSE doctoral programs for September 2024 admission. During the 2023-2024 winter/early spring we conducted our first admission cycle for this new program in conjunction with the admission process for the Dept-CSE PhD program.

While both CSE doctoral programs enable students to specialize at the doctoral level in a computation-related field via focused coursework and a thesis, they differ in essential ways. The standalone CSE PhD program is intended for students who plan to pursue research in cross-cutting methodological aspects of computational science. The resulting doctoral degree in Computational Science and Engineering is awarded by CCSE via the Schwarzman College of Computing. In contrast, the interdisciplinary Dept-CSE PhD program is intended for students who are interested in computation in the context of a specific engineering or science discipline. For this reason, this degree is offered jointly with participating departments across the Institute; the interdisciplinary degree is awarded in a specially crafted thesis field that recognizes the student's specialization in computation within the chosen engineering or science discipline. Applicants to the standalone CSE PhD program are expected to have an undergraduate degree in CSE, applied mathematics, or another field that prepares them for an advanced degree in CSE while applicants to the Dept-CSE PhD program should have an undergraduate degree in a related core disciplinary area as well as a strong foundation in applied mathematics, physics, or related fields.

## COMPUTATIONAL SCIENCE & ENGINEERING DOCTORAL PROGRAMS (CSE PHD & CSE-DEPT PHD)

The interdisciplinary doctoral program in computational science and engineering (Dept-CSE PhD), established in 2013, is administered jointly by CCSE and the participating departments, namely the Departments of Aeronautics and Astronautics, Chemical Engineering, Civil and Environmental Engineering, Earth, Atmospheric and Planetary Sciences, Materials Science and Engineering, Mathematics, Mechanical Engineering and Nuclear Science and Engineering.

Enrollment in the Dept-CSE PhD program at the start of AY2024 included 69 students, 13 of whom matriculated in September 2023, with an additional seven current doctoral students in affiliated home departments joining over the course of the academic year. Two Dept-CSE PhD students graduated in September 2023, three graduated in February 2024, and nine graduated in May 2024, bringing the Dept-CSE PhD alumni total to 96.

The admissions committee for September 2024 CSE doctoral programs was co-chaired by the CCSE co-directors, Nicolas Hadjiconstantinou (Mechanical Engineering) and Youssef Marzouk (Aeronautics and Astronautics). It also included Profs. Laurent Demanet (Mathematics), Raul Radovitzky (Aeronautics and Astronautics), Tess Smidt (Electrical Engineering and Computer Science), and Wim van Rees (Mechanical Engineering). The programs received a total of 411 applications for September 2024 admission; 161 to the joint Dept-CSE PhD program and 250 to the new standalone CSE PhD program. Consistent with past years, the Dept-CSE PhD applicants were first reviewed by the CSE committee and subsequently admissible applicants were shared with the relevant department(s) for consideration and final admission decisions. The process of sharing applications was conducted internally via Slate for the six participating departments also using the software, a considerable improvement over the email-based process used in previous years when admissions was handled using the GradApply software. Ultimately, seven applicants were admitted to the joint program with five accepting and anticipated to enroll in September 2024. Admission decisions for the standalone program were at the sole discretion of the CCSE committee, with ten applicants offered admission and four accepting and expected to enroll in September 2024.

### **COMPUTATIONAL SCIENCE & ENGINEERING MASTER OF SCIENCE PROGRAM (CSE SM)**

Enrollment in the CSE SM program at the start of AY2024 was 25 students, 12 of whom were entering first-year students. Three CSE SM students graduated in September 2023, one in February 2024 and five graduated in spring 2024, increasing the total number of SM alumni to 216. To focus our recruiting efforts and student funding on our new CSE PhD program, we paused external admissions for the CSE SM degree for September 2024.

### **RELOCATION TO BUILDING 45**

As the final step transitioning from the School of Engineering to the College of Computing, CCSE moved from SoE space on the fourth floor of Building 35 to a suite on the fourth floor of the College's new Building 45 on November 6, 2023, during phase one of the building move in. Other phase one occupants included the College Dean's Office and additional smaller units with assigned spaces on the third and fourth floors. In the new space, suite 421, CCSE has 4 private offices, desk space for students and postdocs, and a small social area including a couch, armchair and communal table. Currently the administrative offices for the MIT-IBM Watson AI Lab are also co-located in suite 421. As construction in the building continued through early January 2024, phase one occupants assisted with troubleshooting building facilities and provided feedback that allowed phase two occupants on floors five, six and seven a smoother transition to the building in January 2024.

### **STAFFING UPDATE**

We are excited to report we were able to use carry forward budgetary resources to temporarily fund a full time senior academic assistant position. Ms. Zhao Xian joined CCSE in the role on October 16, 2023 and has since taken over managing CCSE's physical space, coordinating CCSE's seminars, collecting student funding information, soliciting and entering thesis research grades, assisting with event planning, updating and maintaining CCSE's website, and interfacing with CCSE's student group, the Association of Computational Science and Engineering Students (ACES) as well as serves as CCSE's Digital Accessibility Liaison among other duties.

## CCSE COMMUNITY EVENTS & ACTIVITIES

With the addition of a full-time staff member and the availability of more physical spaces in the new building, CCSE was able to increase the number of community events and activities offered in the winter and spring of 2024, an important step in our efforts toward building a stronger CCSE community.

In conjunction with the MindHandHeart (MHH) initiatives and events, CCSE celebrated Random Act of Kindness (RAK) Week March 11 - 15, 2024 by hosting events in the CCSE suite and adjacent spaces and providing an assortment of refreshments and small giveaways throughout the week.

On March 21, 2024 CCSE hosted newly admitted CSE PhD and Dept-CSE PhD students for a campus visit and open house. Activities included an info session and Q&A with Prof. Youssef Marzouk, CCSE Co-Director, and Kate Nelson, CCSE Academic Administrator, presentations from MIT Housing & Residential Services (HRS) and MIT Office of Research Computing and Data (ORCD), a panel discussion featuring current students, including lunch with the panelists, a campus tour lead by current students and open office hours. That evening CCSE hosted its first community reception open to all CCSE affiliates from admitted students through alumni, faculty, staff and postdocs. The event was CCSE's first to take place in the new conference space on the eighth floor of Building 45 and with close to 100 attendees enjoying the evening it was a success.

In collaboration with MIT's Office of Graduate Education (OGE), CCSE celebrated Graduate Student Appreciation Week April 1 - 7, 2024 with additional gatherings, giveaways and refreshments. Both RAK week and Grad Appreciation week events were well attended with students commenting that they appreciated the opportunity to connect with other CCSE-affiliated students from across the Institute.

On May 2, 2024 CCSE held the first faculty luncheon in Building 45 with the agenda covering CCSE updates, a review of the most recent admissions cycle, updates regarding the development of a CSE Common Ground program of study and planning for the 2024-25 academic year.

Also during spring 2024 CCSE submitted a proposal, "Growing the Computational Science and Engineering (CSE) academic community at MIT", to the Chan Wui and Yunyin Retreat Fund through the College requesting support for a full day retreat to foster community and interconnectedness as well as focus on academic and professional development of CCSE students and postdocs and facilitate forward-looking discussions regarding CSE research and research collaborations. In late April we were notified that the proposal was selected for funding. Planning for the event is currently underway with a proposed date of October 15, 2024.

## CCSE SEMINARS

### 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 2023–2024 talks were all conducted in person, with spring talks taking place adjacent to the CCSE suite in Building 45, and recorded via Zoom webinar with captioned recordings available on the [CCSE YouTube channel](#). Below is the list of invited speakers and topics from this past year:

- Laure Zanna, Professor of Mathematics & Atmosphere/Ocean Science, New York University, "A New Generation of Global Climate Models Augmented by AI"

- John Evans, Associate Professor, Jack Rominger Faculty Fellow, Ann and H.J. Smead Department of Aerospace Engineering Sciences, University of Colorado Boulder, “Immersed Finite Element Methods: Opportunities, Challenges, and Recent Advances”
- Yannis Kevrekidis, Bloomberg Distinguished Professor at John Hopkins University and Pomeroy and Betty Perry Smith Professor (Emeritus) at Princeton University, “No Equations, No Variables, No Space and No Time: Data and the Modeling of Complex Systems”
- Lexing Ying, Professor of Mathematics, Stanford University, “Eigenmatrix for Unstructured Sparse Recovery”
- Yunan Yang, Goenka Family Assistant Professor in Mathematics, Cornell University, “When Optimal Transportation Meets PDE-Based Inverse Problems”
- Pep Español, Full Professor in Applied Physics, Universidad Nacional de Educación a Distancia in Madrid, “Stochastic Dissipative Euler's Equations”

### CSE COMMUNITY SEMINARS

Positioned differently from the Distinguished Seminars in CSE, this seminar series focuses on internal speakers (current grad students, post-docs, researchers, and faculty) or informal visits by external CSE-focused researchers (ranging from grad students to faculty). The objectives for this seminar are:

- To strengthen our community among all people at MIT engaged in CSE
- To encourage interdisciplinary dissemination of CSE research across MIT
- To provide an opportunity for early career CSE researchers to present their work, including as practice prior to presenting at conferences, job talks, etc.

This weekly seminar series complements CCSE’s Distinguished Seminar Series which occurs monthly and similarly attracts enthusiastic groups of graduate students, researchers and faculty, sparking heightened interest in CSE research dissemination and discussions. These seminars effectively blend rigorous academic exchanges with community building. Below is a list talks delivered since the start of the series in April 2024:

- Tess Smidt, X-Window Consortium Professor, Assistant Professor in Electrical Engineering, MIT EECS, “Harnessing The Properties of Equivariant Neural Networks To Understand And Design Atomic Systems” (in person)
- Adrian Lozano-Duran, Draper Assistant Professor, MIT Aeronautics and Astronautics, “Causal inference in complex physical systems” (in person)
- Hamid R. Karbasian, Postdoctoral Research Associate, MIT Mechanical Engineering, “AI for Design: unsteady prediction of a dynamical system in the parametric design space” (in person)
- Olivier Zahm, Research Scientist, Inria (the French National Research Institute for Digital Science and Technology), “Sequential transport maps using SoS surrogates” (in person)
- Ayoub Belhadji, Postdoctoral Researcher, MIT Uncertainty Quantification Group, “Towards a unified approximation theory using determinantal point processes” (in person)

- Ngoc Cuong Nguyen, Principal Research Scientist, MIT Aeronautics and Astronautics, “Environment-adaptive machine learning potentials for atomistic simulations of materials under extreme conditions” (in person)

## **PROFESSIONAL DEVELOPMENT PROGRAMS**

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

The program launched in April 2020 and has been running continuously since, with multiple offerings in the past academic year.

**Nicolas Hadjiconstantinou, Co-director**  
**Professor of Mechanical Engineering**

**Youssef Marzouk, Co-director**  
**Professor of Aeronautics and Astronautics**

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