Computational Science and Modeling

Academic Year 2023-2024

Topic Description

Computational science is concerned with all questions related to the computer solution of problems from the modeling of natural, social and engineering sciences. At a fundamental level, areas of computational science and modeling research with increasing interconnectedness across Dartmouth College broadly include the study of dynamical systems, optimization, inverse problems and inference, signal and image processing, network analysis, data mining, quantum computing, and machine learning. More generally, computational science and modeling are inherent to a wide variety of scientific disciplines, including the many areas of biology, computer science, climate studies, earth science, engineering, geology, and across the social sciences. Dartmouth faculty engaged in computational science and modeling research regularly receive research funding from a number of research agencies, including the NSF (across the DMS, CISE and ENG directorates) as well as the NIH, DOD, and DOE.

Policymakers make critical decisions with limited information on rapid timescales. Collaborative research between computational scientists and modelers across the campus can help to advance understanding of group dynamics and decision-making in the presence of uncertainty, and to incorporate the influence of social behavior into scientific models, which can in turn be numerically simulated. Predictive science (independent of social behavior) also needs to be advanced to better understand future risks and enable better planning.

The goal of this seminar series is to bring people together who offer perspective on and are interested in nurturing and developing broad-based collaborations in research and training. This seminar is notably not about discussing individual research projects. In particular, a major theme for the seminar series is to discuss how researchers from seemingly different parts of campus can create more tightly woven research and training opportunities in computational science and modeling, and how to leverage our combined resources and expertise to improve the training of the next generation of computational scientists. The following themes will serve as our touchstones for discussions and to guide possible action items.

1. **Growing recognition in federal funding agencies of the importance of interdisciplinary research.** As an example, we can look to the recently passed CHIPS and Science Act, which authorizes approximately 102 billion dollars to advance major research initiatives at NSF, DOE, the National Institute of Standards and Technology (NIST), and NASA. It also creates a new bioeconomy research and development national initiative, and establishes Regional Technology Hubs. In particular the legislation authorizes 81 billion dollars to the NSF over five years, growing annual authorized funding to 19 billion dollars in FY 2027. Of the key technology areas included in the legislation, computational science and modeling relevant areas include artificial

intelligence (AI) and machine learning; high performance computing; disaster prevention and mitigation; biotechnology and synthetic biology; data management and cybersecurity; advanced materials science; and advanced energy and efficiency technologies

2. **Training our students for next generation challenges.** Broad-based knowledge in computational science and modeling will become increasingly important in solving the challenging problems of the future. For example, climate change presents myriad complex challenges. It is therefore essential that students in this realm be prepared to work effectively on diverse, multidisciplinary, convergent teams, including with social scientists. This requires continued and growing university investments in computational science and modeling education.

3. **The seminar will also discuss how to increase diversity, equity, and inclusion in the field of computational science and modeling.** A key question will be whether an interdisciplinary degree program at the undergraduate and graduate level is needed at this time, and how the Neukom Center and other resources on campus can be leveraged to generate the best outcomes.

Membership

- Anne Gelb and Peter Mucha (Department of Mathematics) will organize and convene the seminar.

From the Sciences Departments of:

- Biological Sciences;
  James O'Malley
- Chemistry;
  Jacquelyne Read
- Earth Science;
  Brendan Keller
- Physics and Astronomy;
  Kristina Lynch

From the Interdisciplinary Departments and Programs of:

- Quantitative Social Sciences;
  Herbert Chang

As well as:

- Thayer School of Engineering;
  Peter Chin
  Colin Meyer
  Don Perovich (affiliate EAS)
  Eugene Santos (affiliate CS)

- Tuck School of Business;
  Jim Smith
  Raghav Singal