# AI for Scientific Discovery - A Workshop

## Committee

## Bradley A. Malin

**Co-Chair**

BRADLEY A. MALIN (NAM) is the vice chair for research and professor of biomedical informatics at Vanderbilt University. He is also a professor of biostatistics, a professor of computer science, and is affiliated faculty in the Center for Biomedical Ethics and Society. He co-directs the Health Data Science (HEADS) Center, the Center for Genetic Privacy and Identity in Community Settings (GetPreCiSe)—a National Institutes of Health (NIH) Center of Excellence in Ethical, Legal, and Social Implications Research (CEER), and the Big Biomedical Data Science Ph.D. program. He is also the director of the Health Information Privacy Laboratory (HIPLab), which was established to address the growing need for data privacy research and development for the health information technology sector. Dr. Malin’s research is in big health data analytics and the infrastructure necessary to support such investigations. He has made specific contributions to a number of health-related areas, including distributed data processing methods for medical record linkage and predictive modeling, intelligent auditing technologies to protect electronic medical records from misuse in the context of primary care, and algorithms to formally anonymize patient information disseminated for secondary research purposes. He is an elected fellow of the National Academy of Medicine and American College of Medical Informatics and was honored as a recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE). Dr. Malin completed his education at Carnegie Mellon University, where he received a bachelor's in biological sciences, a master's in machine learning, a master's in public policy and management, and a doctorate in computer science (with a focus on databases and software systems).

## Keith Andrew Brown

**Member**

Keith A. Brown is an Associate Professor of Mechanical Engineering, Physics, and Materials Science & Engineering, at Boston University. Keith runs an experimental research group that studies polymers with a major focus on accelerating materials research using self-driving labs, transformative formats for experiments, and machine learning. Keith has been a leader in the AI-accelerated materials research community and currently chairs the AI for materials development staging group of the Materials Research Society in addition to service to the Acceleration Consortium. Keith has co-authored over 90 peer-reviewed publications, six issued patents, and his work has been recognized through awards including the Frontiers of Materials Award from The Minerals, Metals, & Materials Society (TMS), being recognized as a “Future Star of the AVS,” the Omar Farha Award for Research Leadership from Northwestern University, and the AVS Nanometer-Scale Science and Technology Division Postdoctoral Award. He earned an S.B. in Physics from MIT, a Ph.D. in Applied Physics at Harvard University with Robert M. Westervelt, and was an International Institute for Nanotechnology postdoctoral fellow with Chad A. Mirkin at Northwestern University.

## Missy Cummings

**Member**

Professor Mary (Missy) Cummings received her B.S. in Mathematics from the US Naval Academy in 1988, her M.S. in Space Systems Engineering from the Naval Postgraduate School in 1994, and her Ph.D. in Systems Engineering from the University of Virginia in 2004. A naval officer and military pilot from 1988-1999, she was one of the U.S. Navy's first female fighter pilots. She is a Professor in the George Mason University College of Engineering and Computing and is the director of the Mason Autonomy and Robotics Center. She is an American Institute of Aeronautics and Astronautics Fellow, and recently served as the senior safety advisor to the National Highway Traffic Safety Administration. Her research interests include the application of artificial intelligence in safety-critical systems, assured autonomy, human-systems engineering, and the ethical and social impact of technology.

## Yolanda Gil

**Member**

Dr. Yolanda Gil is Principal Scientist and Senior Director for Strategic Initiatives in Artificial Intelligence and Data Science at the Information Sciences Institute of the University of Southern California, Director of AI and Data Science Initiatives in the Viterbi School of Engineering, and Research Professor in Computer Science and in Spatial Sciences. She received her M.S. and Ph. D. degrees in Computer Science from Carnegie Mellon University, with a focus on artificial intelligence and cognitive science. Dr. Gil collaborates with scientists in many domains on semantic workflows and metadata capture, provenance and trust, social knowledge collection, computer-mediated collaboration, and automated discovery. In 2019 she co-chaired the CRA/AAAI 20-Year Artificial Intelligence Research Roadmap for the US with key strategic recommendations based on extensive community engagement. She is a Fellow of the Association for Computing Machinery (ACM), the Association for the Advancement of Science (AAAS), and the Institute of Electrical and Electronics Engineers (IEEE). She is also Fellow of the Association for the Advancement of Artificial Intelligence (AAAI) and served as its 24th President. In 2022, she received the M. Lee Allison Award for Outstanding Contributions to Geoinformatics and Data Science from the Geological Society of America (GSA).

## Patrick Francis Riley

**Member**

Patrick Riley leads the artificial intelligence group at Relay Therapeutics, applying learning methods to the discovery process. He has over 15 years of data science and machine learning experience. He came to Relay Therapeutics from Google, where he was a principal software engineer and a lead of the Accelerated Science team. His work spanned areas as diverse as cell imaging, nuclear fusion and materials science. His most important work was on the application of machine learning to small molecules, including foundational work on graph neural networks and their application to DNA encoded small molecule library screening.

Patrick holds a Ph.D., M.S. and B.S. in Computer Science from Carnegie Mellon University.

## Aarti Singh

**Member**

Dr. Singh is a tenured associate professor in the Machine Learning Department at Carnegie Mellon University. Her research lies at the intersection of machine learning, statistics, and signal processing, and focus on designing statistically and computationally efficient algorithms that can leverage inherent structure of the data using direct, compressive and interactive queries. She received a B.E. in electronics and communication engineering from the University of Delhi, and a M.S. and Ph.D. in electrical engineering from the University of Wisconsin-Madison. Prior to her position at CMU, Dr. Singh was a postdoctoral research associate at the Program in Applied and Computational Mathematics at Princeton University. Her work is recognized by an NSF Career Award, a United States Air Force Young Investigator Award, A. Nico Habermann Junior Faculty Chair Award, Harold A. Peterson Best Dissertation Award, and four best student paper awards. Her service honors include serving as program chair for the International Conference on Machine Learning (ICML) 2020, program chair for Artificial Intelligence and Statistics (AISTATS) 2017 conference, associate editor for IEEE Transactions of Information Theory and IEEE Transactions on Signal and Information Processing over Networks, steering committee for an NSF innovation lab, and the National Academy of Sciences (NAS) committee on Applied and Theoretical Statistics.

## Alex Temple

**Staff Officer**

Alex Temple is a Program Officer at the National Academy of Sciences, Engineering, and Medicine (NASEM). Alex works to bring scientists, government leaders, and industry experts together to discuss pressing scientific issues. Prior to NASEM, Alex worked at the U.S. Department of State in the Office of Science and Technology Cooperation where he covered Africa, Science and technology Agreements, and innovation programming activities. Alex specializes in science diplomacy, capacity building, and convening of scientists. Alex earned his bachelors at The Ohio State University, a Masters from Carnegie Mellon University, and it currently pursuing a PhD at George Washington University in Science and Technology Policy.