

Foundation Models for Scientific Discovery and Innovation: Opportunities Across the Department of Energy

Committee

Dona L. Crawford

Chair

Dona L. Crawford retired as associate director for computation from the Lawrence Livermore National Laboratory (LLNL), where she led the laboratory's high-performance computing efforts. In that capacity, Ms. Crawford was responsible for the development and deployment of an integrated computing environment for petascale simulations of complex physical phenomena. Prior to her LLNL appointment in 2001, Ms. Crawford was with Sandia National Laboratories (SNL) since 1976 serving on many leadership projects including the Accelerated Strategic Computing Initiative and the Nuclear Weapons Strategic Business Unit. Ms. Crawford serves on the National Academies Laboratory Assessments Board and has previously served on several NASEM committees including the Committee to evaluate Post-Exascale Computing for the National Nuclear Security Administration, the Committee to Review Governance Reform in the National Nuclear Security Administration and the Committee to Evaluate the NSF's Vertically Integrated Grants for Research and Education (VIGRE) Program. She received her MS in operations research from Stanford University.

Syed Bahauddin Alam

Member

Dr. Syed Bahauddin Alam is an Assistant Professor of Nuclear, Plasma, & Radiological Engineering at the University of Illinois Urbana-Champaign (UIUC), where he leads the MARTIANS (Machine Learning & ARTificial Intelligence for Advancing Nuclear Systems) Laboratory. He holds a joint appointment at the National Center for Supercomputing Applications. Previously, he served as a faculty at Missouri S&T, was a Nonproliferation Fellow at KAIST, and held MeV Fellowship at Argonne National Laboratory. Dr. Alam's research expertise centers on explainable AI and data science, with a primary focus on developing real-time AI algorithms for nuclear energy systems. His innovative contributions to digital twins and advanced reactors have integrated cutting-edge AI methodologies, enhancing safety and efficiency through real-time predictive capabilities. He has been recognized with numerous prestigious awards, including the Illinois Innovation Award finalist for excellence in cutting-edge innovation, a "Top of Minds" feature by UIUC Grainger College, the Cambridge Philosophical Society Award for an exceptionally promising piece of research, American Nuclear Society Best Paper Award, the Cambridge Trust Award, and an Outstanding Teaching Award. He earned his Ph.D. (2018) and MPhil (2013) in Nuclear Engineering from the University of Cambridge and previously conducted postdoctoral research at the French Atomic Energy Commission.

Marta D'Elia

Member

Marta D'Elia is the Director of AI and ModSim at Atomic Machines and an Adjunct Professor at Stanford University, ICME. She previously worked at Pasteur Labs, Meta, and Sandia National Laboratories as a Principal Scientist and Tech Lead. She holds a PhD in Applied Mathematics and master's and bachelor's degrees in Mathematical Engineering. Her work deals with design and analysis of machine-learning models and optimal design and control for complex industrial applications. She is an expert in nonlocal modeling and simulation, optimal control, and scientific machine learning. She is an Associate Editor of SIAM and Nature journals, a member of the SIAM industry committee, the Vice Chair of the Siam Northern California section, and a member of the NVIDIA advisory board for scientific machine learning.

Krishna Garikipati

Member

Krishna Garikipati obtained his PhD at Stanford University in 1996, and after a few years of post-doctoral work, he joined the University of Michigan in 2000, rising to Professor in the Departments of Mechanical Engineering and Mathematics. Between 2016 and 2022, he served as the Director of the Michigan Institute for Computational Discovery & Engineering (MICDE). In January 2024 he moved to the Department of Aerospace and Mechanical Engineering at University of Southern California. His research is in computational science, with applications drawn from biophysics, materials physics, mechanics and mathematical biology. Of recent interest are data-driven approaches to computational science. He has been awarded the DOE Early Career Award for Scientists and Engineers, the Presidential Early Career Award for Scientists and Engineers (PECASE), and a Humboldt Research Fellowship. He is a fellow of the US Association for Computational Mechanics, the International Association for Computational Mechanics, and the Society of Engineering Science, a Life Member of Clare Hall at University of Cambridge, and a visiting scholar in Computational Biology at the Flatiron Institute of the Simons Foundation.

Shirley Ho

Member

Shirley Ho is a senior research scientist at the Center for Computational Astrophysics at the Simons Foundation and she joined the Foundation in 2018 to lead the Cosmology X Data Science group. Her research interests range from cosmology to developing new machine learning methods for scientific data that leverage shared concepts across scientific domains. Ho has extensive expertise in astrophysical theory, observation, and data science. She focuses on novel statistical and machine learning tools to address cosmic mysteries like the origins and fate of the universe. Ho analyzes data from surveys including ACT, Euclid, LSST, Simons Observatory, SDSS, and Roman Space Telescope to understand our universe's evolution. She earned her Ph.D. in Astrophysical Sciences from Princeton in 2008 and B.S. degrees in Computer Science and Physics from UC Berkeley in 2004. Ho was previously a Chamberlain and Seaborg Fellow at Lawrence Berkeley National Lab. She joined Carnegie Mellon as an Assistant Professor in 2011, becoming Cooper Siegel Career Development Chair Professor and tenured Associate Professor. In 2016 she moved to Lawrence Berkeley Lab as a Senior Scientist.

Scott H. Holan

Member

Dr. Scott H. Holan is a Professor of Statistics and Department Chair at the University of Missouri and serves as a Senior Research Fellow in the Research and Methodology Directorate at the U.S. Census Bureau. His research expertise includes developing statistical and machine learning methodology for dependent data (spatial, spatio-temporal, functional, and multivariate, among others), Bayesian methods, environmental and ecological statistics, official statistics, and survey methodology. He is an elected Fellow of the American Statistical Association (2014), an Elected Member of the International Statistical Institute (2017), and an elected Fellow of the Institute of Mathematical Statistics (2021). Prof. Holan was a previous co-awardee of the Statistical Partnerships Among Academe, Industry, and Government (SPAIG) Award (2017). Prof. Holan has an M.S. in mathematics from University of Illinois at Chicago (1999) and a Ph.D. in Statistics from Texas A&M University (2004).

Michael Kearns

Member

Michael Kearns is professor and National Center Chair of the Department of Computer and Information Science at the University of Pennsylvania and the Founding Director of the Warren Center for Network and Data Sciences. His research interests include topics in machine learning, artificial intelligence, algorithmic game theory and microeconomics, computational social science, and quantitative finance and algorithmic trading. Dr. Kearns often examines problems in these areas using methods and models from theoretical computer science and related disciplines. He also often participates in empirical and experimental projects, including applications of machine learning to problems in algorithmic trading and quantitative finance, and human-subject experiments on strategic and economic interaction in social networks. Dr. Kearns spent the decade 1991-2001 in machine learning and AI research at AT&T Bell Labs and in the last 4 years of his appointment was head of the AI department which conducted a broad range of systems and foundational AI work. Dr. Kearns received his undergraduate from the University of California at Berkeley in math and computer science and his Ph.D. in computer science from Harvard University. In 2020, Dr. Kearns joined Amazon Web Services as an Amazon Scholar, focusing on fairness, privacy and other "responsible AI" topics.

Petros Koumoutsakos

Member

Petros Koumoutsakos is Herbert S. Winokur Professor of Engineering and Applied Sciences and Area Chair of Applied Mathematics at Harvard John A. Paulson School of Engineering and Applied Sciences (SEAS). He also currently holds a visiting position at Google DeepMind based in London. He studied Naval Architecture (Diploma-NTU of Athens, M.Eng.-U. of Michigan), Aeronautics and Applied Mathematics (PhD-Caltech). He has conducted post-doctoral studies at the Center for Parallel Computing at Caltech and at the Center for Turbulent Research at Stanford University and NASA Ames. He has served as the Chair of Computational Science at ETH Zurich (1997-2020) and has held visiting fellow positions at Caltech, the University of Tokyo, MIT, the Radcliffe Institute of Advanced Study at Harvard University and he is Distinguished Affiliated Professor at TU Munich. Petros is elected Fellow of the American Society of Mechanical Engineers (ASME), the American Physical Society (APS), the Society of Industrial and Applied Mathematics (SIAM) and the Collegium Helveticum. He is recipient of the Advanced Investigator Award by the European Research Council and the ACM Gordon Bell prize in Supercomputing. He is elected International Member to the US National Academy of Engineering (NAE).

Brian Kulis

Member

Brian Kulis is an associate professor at Boston University, with appointments in the Department of Electrical and Computer Engineering, the Department of Computer Science, the Faculty of Computing and Data Sciences, and the Division of Systems Engineering. From 2019-2023, he was also an Amazon Scholar, working with the Alexa team. Previously, he was the Peter J. Levine Career Development assistant professor at Boston University. Before joining Boston University, he was an assistant professor in Computer Science and in Statistics at Ohio State University, and prior to that was a postdoctoral fellow at UC Berkeley EECS. His research focuses on machine learning, statistics, computer vision, and large-scale optimization. He obtained his PhD in computer science from the University of Texas in 2008, and his BA degree from Cornell University in computer science and mathematics in 2003. For his research, he has won three best paper awards at top-tier conferences---two at the International Conference on Machine Learning (in 2005 and 2007) and one at the IEEE Conference on Computer Vision and Pattern Recognition (in 2008). He was also the recipient of an NSF CAREER Award in 2015.

Daniel I. Meiron

Member

Dan Meiron is currently a professor of Aerospace and Applied and Computational Mathematics. His research interests are primarily in computational fluid dynamics with connections to high performance computing. He also has interests in computational materials science. He received an ScD in applied mathematics at MIT working under Steven A. Orszag. He has participated as part of a recent NASEM study on Exascale Computing.

Nathaniel Trask

Member

Nathaniel Trask recently joined the Mechanical Engineering Department at the University of Pennsylvania after spending eight years as technical staff at Sandia National Laboratories. His research focuses upon developing foundational aspects of scientific machine learning (SciML) for high-consequence engineering settings. By integrating concepts from modern physics and probability into the design of deep learning architectures, he leads a research program both employing SciML for scientific discovery as well as to construct digital twins of complex systems. He is deputy director of SEA-CROGS, an Office of Science funded multi-institutional center developing next-generation AI architectures for Earth and Embedded Systems. He has received the Department of Energy Early Career Award, as well as the National Science Foundation Mathematical Science Postdoctoral Fellowship. His doctoral training was in Applied Mathematics, with a focus on developing novel optimization-based discretizations of partial differential equations to simulate multiphysics and multiscale problems. After moving to Sandia National Laboratories for a fellowship, he went on to work extensively on machine learning applied to material science and physics in extreme environments.

Blake Reichmuth

Staff Officer