Keynote: AI for Scientific Discovery and a Sustainable Future

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KEYNOTE ABSTRACT

Artificial Intelligence (AI) is a rapidly advancing field. Novel machine learning methods combined with reasoning and search techniques have led us to reach new milestones: from computer vision, machine translation, and Go world-champion level play, to self-driving cars. These ever-expanding AI capabilities open exciting avenues for advances in new domains. I will discuss our AI research for advancing scientific discovery for a sustainable future. In particular, I will talk about our research in a new interdisciplinary field, Computational Sustainability, which aims to develop computational models and methods to help balance the environmental, economic, and societal needs for a sustainable future. I will provide examples of computational sustainability problems, ranging from biodiversity conservation to multi-criteria strategic planning of hydropower dams in the Amazon basin and materials discovery for renewable energy materials. I will also highlight our work on AI to accelerate the discovery of new solar fuels materials. In this work, we propose an approach called Deep Reasoning Networks (DRNets), which requires only modest amounts of (unlabeled) data, in sharp contrast to standard deep learning approaches. DRNets reach super-human performance for crystal-structure phase mapping, a core, long-standing challenge in materials science, enabling the discovery of solar-fuels materials. DRNets provide a general framework for integrating deep learning and reasoning for tackling challenging problems. Finally, I will highlight cross-cutting computational themes and challenges for AI.

KEYNOTE SPEAKER BIOSKETCH

Carla Gomes is the Ronald C. and Antonia V. Nielsen Professor of Computing and Information Science and the director of the Institute for Computational Sustainability at Cornell University. Gomes received a Ph.D. in computer science in artificial intelligence from the University of Edinburgh. Her research area is Artificial Intelligence with a focus on large-scale constraint reasoning, optimization, and machine learning. Recently, Gomes has become deeply immersed in research on scientific discovery for a sustainable future and, more generally, in research in the new field of Computational Sustainability. Computational Sustainability aims to develop computational methods to help solve some of the key environmental, economic, and societal challenges to help put us on a path toward a sustainable future. Gomes was the lead PI of two NSF Expeditions in Computing awards. Gomes has (co-)authored over 200 publications, which have appeared in venues spanning Nature, Science, and a variety of conferences and journals in AI and Computer Science, including five best paper awards. Gomes was named the "most influential Cornell professor" by a Merrill Presidential Scholar (2020). Gomes was also the recipient of the Association for the Advancement of Artificial Intelligence (AAAI) Feigenbaum Prize (2021) for "high-impact contributions to the field of artificial intelligence, through innovations in constraint reasoning, optimization, the integration of reasoning and learning, and through founding the field of Computational Sustainability, with impactful applications in ecology, species conservation, environmental sustainability, and materials discovery for energy" and of the 2022 ACM/AAAI Allen Newell Award, for contributions bridging computer science and other disciplines. Gomes is a Fellow of the Association for the Advancement of Artificial Intelligence (AAAI), a Fellow of the Association for Computing Machinery (ACM), and a Fellow of the American Association for the Advancement of Science (AAAS).