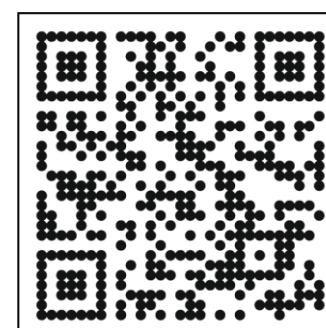




北京大学前沿计算研究中心
Center on Frontiers of Computing Studies, Peking University

静园5号院
前沿讲座



AI4Science: Industrial Applications and Foundation Models for Scientific Discovery



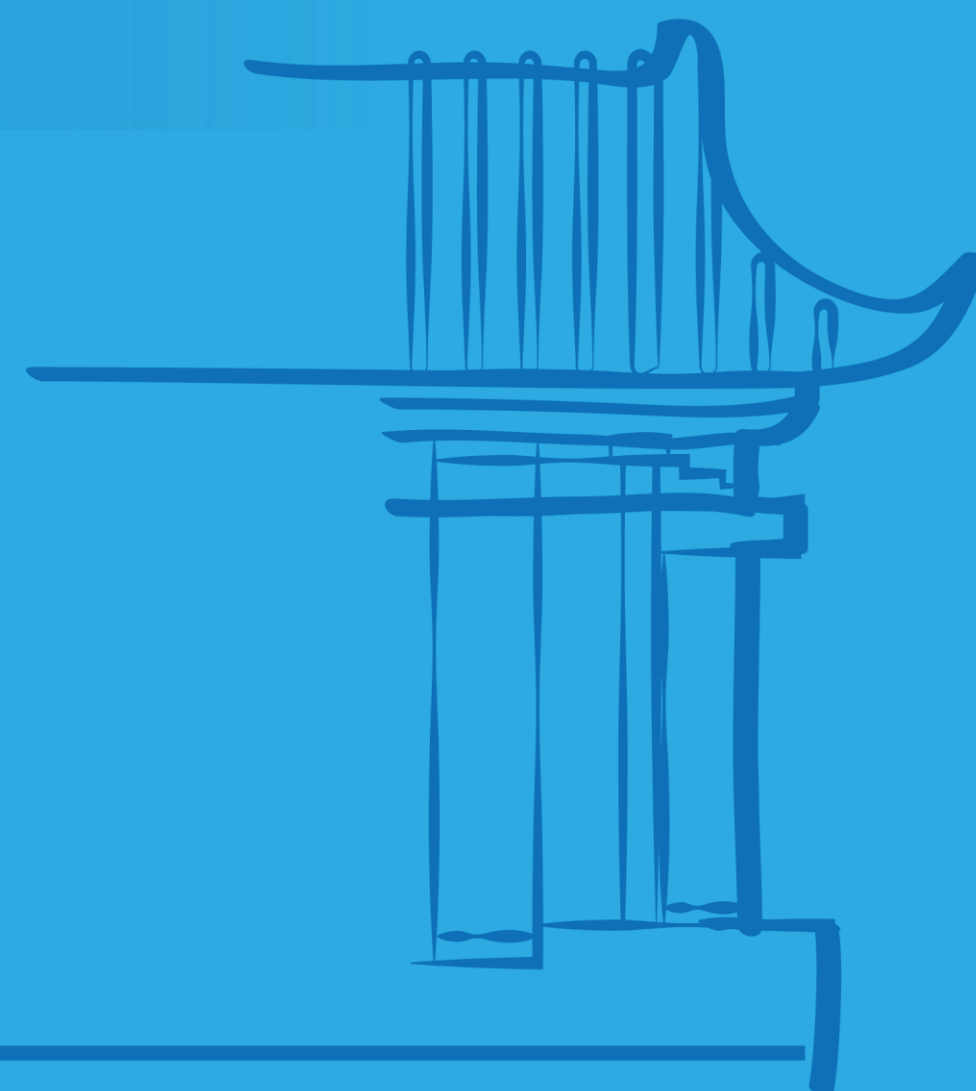
Dr. Kai Liu

Vice President of Artificial Intelligence
SES AI

🎤 Host: 董豪 助理教授

🕒 2025年6月10日 星期二 02:00pm

📍 静园五院204室



Abstract

In recent years, AI for Science (AI4Science) has emerged as a transformative paradigm, driving advances across diverse domains such as drug discovery, materials science, chemical synthesis, mathematics, and machine learning itself. Many of the most pressing scientific questions today are increasingly data-driven—whether arising from molecular graph representations, multi-modal biomedical data, or high-dimensional pathological images. In this landscape, AI is rapidly becoming the “third pillar” of scientific discovery, complementing theoretical reasoning and experimental validation.

In this talk, I will present real-world case studies from industry research, particularly in biotechnology and materials science, to illustrate how AI is reshaping scientific workflows. I will discuss how multi-omics patient data can be mined using machine learning to reveal novel drug targets and enable personalized therapies. I will also highlight how equivariant neural networks can approximate Density Functional Theory (DFT) to accurately predict molecular properties and accelerate material design.

The last part of the talk will focus on the emergence and application of foundation models in scientific domains. I will introduce agentic AI, foundation model applications and several foundation models we developed, especially OmniScience, a text-based large language model (LLM) capable of reasoning over literature and experimental knowledge. I will share insights into how these models can be applied to real-world scientific problems—and how they can be further enhanced to better support hypothesis generation, knowledge reasoning, and discovery acceleration.

Ultimately, I will argue that the future of AI4Science lies in integrating domain-specific data with structured scientific knowledge, enabling machines not just to analyze data, but to think and reason like scientists—fostering breakthroughs that were once the domain of human intuition alone.

Biography

Dr. Kai Liu is a recognized AI4Science leader with over a decade of experience in machine learning, large language models (LLMs), and scientific discovery. As Vice President of Artificial Intelligence at SES AI, he led the AI team in advancing battery materials discovery, including the development of OmniScience, a 70-billion-parameter scientific foundation model that set new standards in domain-specific reasoning. Previously, as Director of Artificial Intelligence at Genentech, Dr. Liu founded and led AI teams focused on multimodal omics learning, immunogenicity prediction, and natural language processing, driving innovation in drug discovery, biomarker development, and clinical trial design. He has published in leading journals and conferences including Nature, Nature Communications, Scientific Reports, and NeurIPS etc. Dr. Liu holds a Ph.D. in Neuroscience and an M.S.E. in Machine Learning from Johns Hopkins University.

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