Plenary Talk 5 by Raphaël Pestourie (School of Computational Science and Engineering at Georgia Tech)

Title: End-to-end optimization from chemistry to environmental physics

Abstract: End-to-end optimization—systematically refining interconnected processes through data-driven models and PDE solvers—is transforming scientific and engineering disciplines. By integrating computational design, machine learning, and physics-based modeling, this framework enables holistic optimization across fields like materials discovery, photonics, and environmental sensing. This talk will explore how end-to-end optimization transcends traditional siloed approaches, leveraging deep learning, inverse design, and multi-fidelity PDE solvers to simultaneously optimize materials, devices, and deployment strategies. Versatile and scalable, this framework unifies data-driven learning with physics-based simulation, driving advances in quantum systems, biomedical imaging, and renewable energy. This talk will highlight how end-to-end optimization bridges fundamental science and real-world impact, accelerating innovation across disciplines.