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FOUNDATION MODELS AND AGENTIC COMPUTATIONAL INTELLIGENCE FOR SCIENTIFIC DISCOVERY AND ENGINEERING

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ABSTRACT

Recent advances in computational intelligence (CI) are transforming computational science through foundation models (FMs) that learn transferable representations across scientific datasets and physical systems. In parallel, agentic CI is enabling new approaches to orchestrating scientific investigations through adaptive decision-making, coordinated use of computational tools, and iterative interactions with simulations and experimental evidence. Together, these developments offer opportunities to move beyond isolated predictive models toward integrated, more reliable, and increasingly autonomous workflows for scientific discovery and engineering.

This invited session will examine the mathematical, algorithmic, and computational foundations of scientific FMs and agentic CI, along with their integration into practical research workflows. Topics include: (i) multi-task and transfer learning across heterogeneous data and physical systems; (ii) physics-informed modeling, (iii) CI agents that coordinate predictive models, (iv) autonomous hypothesis evaluation, and (v) adaptive experiment design.

Particular attention will be devoted to connecting learned representations with established computational methods, including numerical simulation, optimization, and uncertainty-aware decision-making. Contributions addressing robustness, interpretability, physical consistency, computational efficiency, and verification of data-driven scientific conclusions are especially encouraged. Relevant applications include materials science, computational mechanics, climate modeling, and energy systems.