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AGENTIC AI FOR SCIENTIFIC DISCOVERY: INTEGRATING CFD, EXPERIMENTS, AND OBSERVATIONS

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ABSTRACT

Recent advances in Large Language Models (LLMs) and agentic AI systems are transforming the paradigm of scientific research. Traditionally, computational fluid dynamics (CFD), experiments, and observational analyses have been conducted as largely independent processes, requiring substantial manual effort in model development, simulation setup, data interpretation, geometry preparation, and code implementation. Emerging LLM-driven approaches are now enabling these components to be integrated into unified and increasingly automated scientific workflows.

This minisymposium focuses on agentic AI for scientific discovery, with an emphasis on integrating CFD, experiments, and observations. We highlight the role of LLMs not only as tools for analysis but as active components in the research loop, capable of assisting hypothesis generation, simulation orchestration, experimental design, geometric modeling, and coding automation.

Topics of interest include, but not limited to:

(i) LLM-assisted CFD modeling, solver development, and simulation workflows;

(ii) automated code generation, verification, and refactoring for scientific computing;

(iii) AI-driven experimental design and interpretation;

(iv) integration of multimodal data including simulation, experimental, and observational datasets;

(v) agent-based systems enabling closed-loop workflows across simulation and experiments;

(vi) hybrid approaches combining physics-based and data-driven models;

(vii) AI-assisted geometric modeling and representation learning, including neural implicit

representations such as DeepSDF and generative models for complex 3D geometries;

(viii) applications in fluid mechanics, thermal engineering, environmental flows, and semiconductor thermal design.

A central theme is the transition from AI as a supporting tool to AI as an autonomous or semi-autonomous scientific agent coordinating complex research processes. This shift has the potential to accelerate discovery, reduce human workload in routine tasks such as coding, geometry preparation, and data processing, and enable new forms of knowledge integration across traditionally separated domains. In particular, the integration of geometry generation, simulation, and analysis suggests a pathway toward end-to-end automated scientific workflows.

By bringing together researchers from computational mechanics, experimental science, and artificial intelligence, this minisymposium aims to establish a forum for discussing emerging methodologies and future directions toward integrated and automated scientific discovery.

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