

DAC WorkGroup on Scientific AI Agents

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ATHENA: Agentic Team for Hierarchical Evolutionary Numerical Algorithms

Progress in computational science depends on complex numerical workflows that must faithfully encode physical laws, yet translating conceptual insight into reliable code remains a major bottleneck. Although large language models can generate isolated code fragments, they lack the structured reasoning required to design, verify, and iteratively refine complete scientific pipelines. Here we introduce ATHENA, an agentic framework explicitly designed to emulate scientific research modeled as a knowledge-driven contextual bandit process. Its core loop separates conceptual policy from numerical realization through expert-derived conceptual scaffolding, enabling principled diagnosis, reformulation, and repair of computational strategies. Across scientific computing and scientific machine learning tasks, ATHENA autonomously discovers exact analytical solutions, constructs stable numerical solvers, diagnoses ill-posed formulations, and orchestrates hybrid symbolic-numeric workflows. Quantitatively, ATHENA exceeds expert-designed workflows, achieving superhuman accuracy and robustness on canonical benchmarks. By reframing computation as an object of agentic reasoning, our framework enables autonomous orchestration of heterogeneous algorithms across scientific domains. Link to paper: <https://arxiv.org/pdf/2512.03476>

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3:30 – 4:30 PM

127 Hayes-Healy Center and Zoom

<https://notredame.zoom.us/j/3795256579>