

Title: “Agentic AI for Multiphysics code development and simulation”

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Abstract:

Integrated multiphysics codes running on HPC systems form the backbone of NNSA’s modelling and simulation capabilities. At LLNL, agentic AI is proving valuable in strengthening this mission critical foundation across both operational workflows and early-stage research. In this talk, we present several examples and share the guiding principles that shape how we apply these tools. On the production side, agentic AI supports code development, debugging, and performance optimization for large scale multiphysics applications. We highlight interaction modes that range from AI assisted algorithm design to fully agentic refactors, including GPU kernel tuning for performance critical regions. We also describe emerging efforts to use agentic AI to help drive simulations, both as a problem setup assistant and as part of an agent-based design optimization loop. Finally, we summarize ongoing work in our research and development of differentiable multiphysics codes for inverse design. Differentiable simulations can serve as physics-based world models, enabling AI agents to explore high dimensional multiphysics design spaces more efficiently.

Bio: