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AGENTIC AI APPLICATIONS IN COMPUTATIONAL MECHANICS: MATERIALS MODELLING AND CHARACTERIZATION

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ABSTRACT

The emergence of large language models and agentic AI frameworks is reshaping the way engineers design, model, and simulate. While AI has already been significantly and widely applied in computational mechanics, from surrogate modelling and topology optimization to data-driven constitutive laws, the advent of autonomous agent systems opens qualitatively new possibilities. Agentic AI is not merely another tool within existing workflows; it represents a shift toward systems that can reason, plan, and act across complex multi-step tasks with minimal human intervention.

Agentic AI offers new possibilities across materials modelling and characterization. By combining the generative and reasoning capabilities of LLMs with physics-based FEM engines and reduced-order models, these systems can automate and orchestrate modelling workflows that previously demanded deep expert knowledge, simplifying model setup and configuration, enabling new approaches to the development of material subroutines and user-defined models, and assisting in parameterization, geometry creation, mesh generation, solver selection, and post-processing.

Beyond workflow automation, autonomous agents open new frontiers in materials characterization: driving inverse identification of material parameters from experimental data, interpreting multimodal geometry inputs for FEM preprocessing, and interfacing with simulation environments through natural language, lowering barriers for non-specialist users while accelerating the expert throughput.

Contributions to this session will cover agentic architectures for simulation, LLM-driven modelling assistants, automated characterization pipelines, automated end-to-end modelling workflows, uncertainty management, and trust in autonomous simulation systems.