

Integrating AI into nanoHUB: Toward Intelligent and Connected Scientific Workflows

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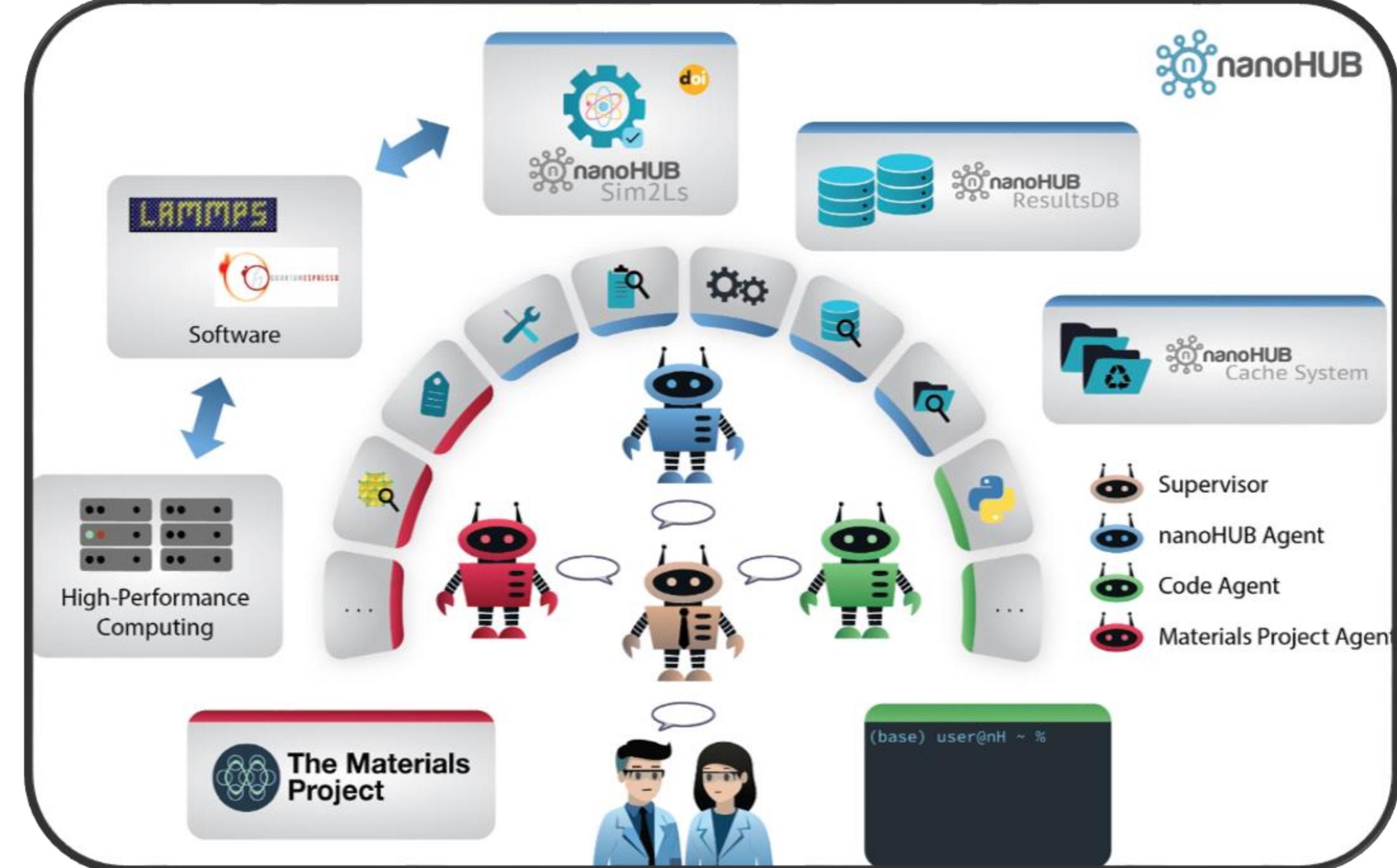
MOTIVATION

AI is reshaping scientific collaboration by integrating distributed knowledge, automating reasoning, and guiding experimentation^{1,2,3}.

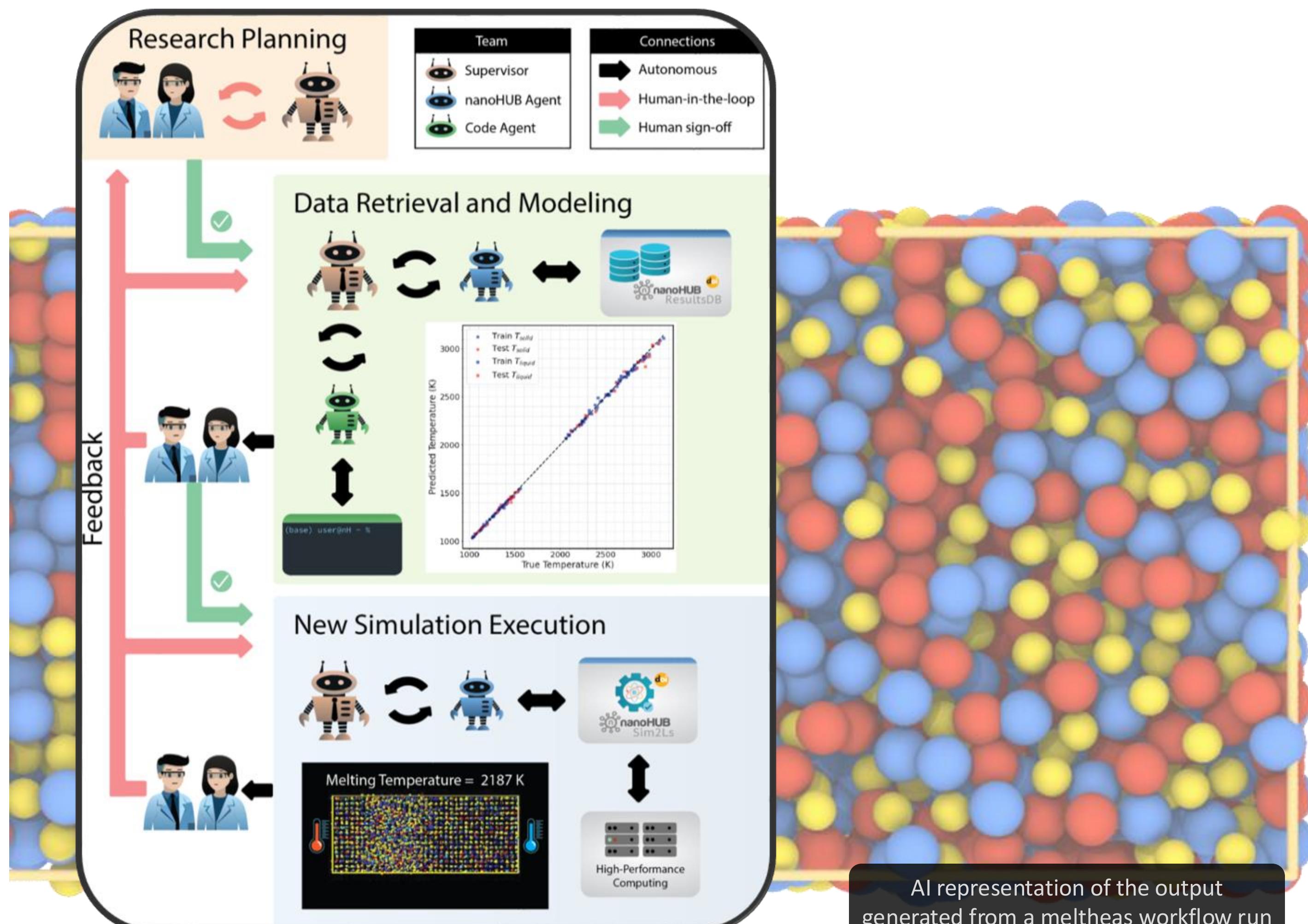
Integrating these technologies into nanoHUB⁴ expands the platform's role from hosting simulations, to enabling intelligent, data-driven workflows.

AI-Driven Scientific Workflows

NanoRA is an agentic AI system that leverages a team of independent agents powered by LLMs to solve scientific endeavors.



Each agent has its own tools to plan, select, and run scientific workflows. Powered by nanoHUB tools and the resultsDB, it uses standardized end-to-end simulation workflows with validated metadata and more than **1,500,000** stored simulation records.



An interactive agentic AI assistant that enables users to discover and explore scientific resources conversationally. It exposes the content as queryable records, storing more than **500,000** semantically searchable data entries.

AI-Enhanced Content Discovery

NanoBUD integrated AI-assisted features that processed more than **8,500** curated resources made up of videos, documents, and tools. It extracted transcripts, abstracts, and tags from content and built a knowledge graph with over **150,000** relations.

CONCLUSIONS

By integrating AI, nanoHUB reshapes the way users explore scientific content, simplifying access to complex tools and enabling understanding through natural, intuitive conversations.

Together, these systems create a seamless experience: nanoCHAT guides users through dialogue, nanoRA runs and interprets simulations, and the platform's AI connects data, tools, and results into one unified environment.

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