



Considerations

When Designing and Building Agentic LLM Systems for Scientific Workflows



Operational and Business Considerations

Technical debt

- It often costs more to integrate and manage new technology than develop it. LLM systems are easy to plug in, but difficult to monitor and upgrade.

Reliability

- LLM systems work “some to most of the time”. They are inherently guessing what to do next, which creates variability in their answers., impacting reproducibility also.

API/token costs

- LLM systems may offer much promise, but the LLM providers make significant money every month if token requests are not managed carefully. Submitting long prompts and publications to LLMs could use a lot of tokens!

Adaptability to new technologies

- This year it is all about agentic systems, next year it will be something else. And the models themselves are advancing rapidly, making the balance between systems design and LLM choice very dynamic. P.S. Many of the advancements seem big but are incremental.

Technical Considerations

Lack of true reasoning and understanding

- Agentic AI systems and LLMs in general rely on probability-driven outputs rather than genuine comprehension or reasoning.

Potential for hallucinations and incorrect outputs

- LLMs are prone to generating "hallucinations," where the model produces information that appears factual but is inaccurate. In an agentic system, this can lead to incorrect autonomous decisions and actions.

Challenges with transparency and accountability

- Agentic AI systems often operate as black boxes, making it difficult to trace the rationale behind their decisions. Chain-of-Thought behavior is improving this.

Biases in decision-making

- Since LLMs are trained on large datasets (mainly from the internet, they may inherit biases present in the data. They may also inherit biases when leveraging publications (RAG databases).

How can the
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help you address these issues?



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