

Computational Molecular Biology and Bioinformatics

Virtual Lab

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Background

Agentic AI refers to AI systems that can act autonomously. Such systems do not just respond to instructions, but can set goals, make plans, and take actions on their own to achieve specific outcomes.

Sometimes, human can also be brought into such AI based systems.

What is Virtual Lab?

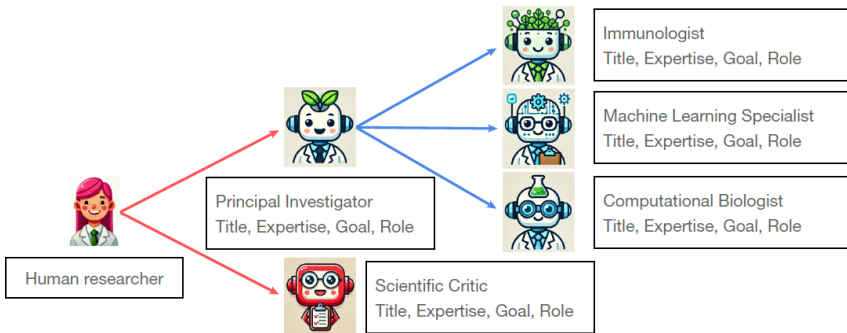
Virtual Lab is an AI-human collaboration to perform sophisticated and interdisciplinary scientific research [1]. The Virtual Lab consists of an LLM Principal Investigator agent guiding a team of LLM scientist agents through a series of research meetings, with a human researcher providing high-level feedback.

Virtual Lab architecture

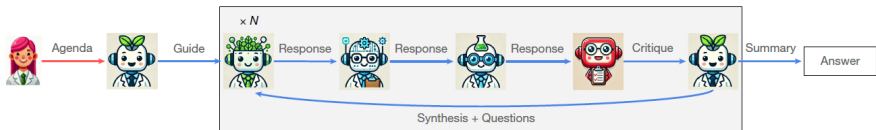
The basic components of Virtual Lab are as follows:

- **Agents:** Each LLM agent is defined with a prompt that specifies (1) Title, the name of the agent; (2) Expertise, the scientific expertise the agent has; (3) Goal, the ultimate goal of the agent in the context of the research project; and (4) Role, the specific role that the agent will play in the research project.
- **Meetings:** Each interaction is defined with Agenda, Agenda questions, Agenda rules, Summaries, Contexts, Rounds. The meetings can be of three types as listed below.
 - **Team meeting**
 - **Individual meeting**
 - **Parallel meetings**

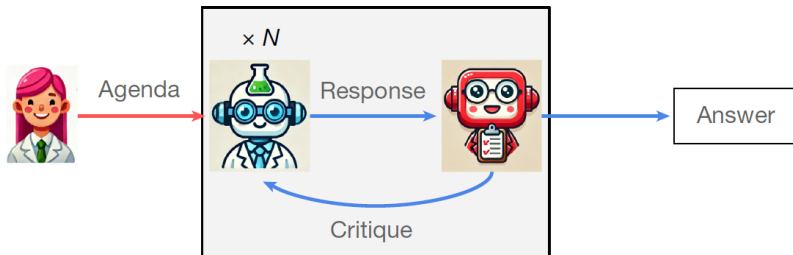
Workflow of Virtual Lab - Designing agents



Workflow of Virtual Lab - Organizing team meetings



Workflow of Virtual Lab - Organizing individual meetings



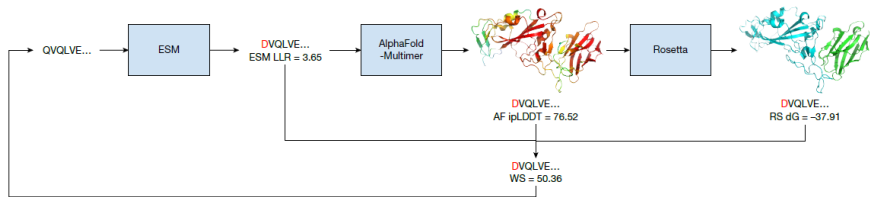
Virtual Lab for nanobody design

Virtual Lab was applied to nanobody design in five phases using GPT-4o (gpt-4o-2024-08-06) as the underlying LLM powering the agents. The following steps were taken up for this.

- Team selection
- Project specification
- Tools selection
- Tools implementation
- Workflow design

Virtual Lab for nanobody design

Each round of nanobody design begins with ESM computing LLRs of single point mutations to the input sequence. For the top 20 mutant sequences by ESM LLR, AlphaFold-Multimer predicts the structure of the nanobody and SARS-CoV-2 spike protein and computes the AF ipLDDT. Rosetta relaxes the complex and computes the RS dG. The top five mutant nanobodies are selected via a WS for the next round of optimization.



References

- 1 Swanson, K., Wu, W., Bulaong, N.L., Pak, J.E. and Zou, J., The Virtual Lab of AI agents designs new SARS-CoV-2 nanobodies. *Nature*, 646:716-723, 2025.