WASP Project Course 2025

A multi-agent system for drug discovery

Background

In chemistry and in drug discovery, several recent publications have demonstrated that it is possible to streamline common tasks, discover new molecules and materials, and integrate into robotics environments by building agents that are powered by large language models (LLMs). Such agents typically augment the reasoning capabilities of the LLMs with external tools and databases. To enable flexibility and scalability, it is advantageous that such systems are multi-agent systems, where specialized agents communicate in some specified workflow to solve a common task.

In this course we will take a practical approach and develop a multi-agent system that can solve tasks in drug discovery. The students will initially work in small groups, where each group is responsible for building a specific agent. Such agents could include one capable of generating novel compounds using the Reinvent tool from AstraZeneca, one capable of looking up chemical information in publicly available databases, and one capable of generating Python code to perform simple cheminformatic tasks, to mention a few. When the individual agents are built, the students will explore multi-agent workflows to connect the individual agents and evaluate their capacity, scalability, and emergent properties. We will use local, open-source LLMs that are served from software such as ollama or llama.cpp. Students will be encouraged to take inspiration from existing publications and open-source codes in developing their multi-agent system.

Constraints: None

Participants

Industrial partner: AstraZeneca

Industrial supervisor: Samuel Genheden, samuel.genheden@astrazeneca.com

Academic supervisor: Richard Johansson, richard.johansson@cse.gu.se, Chalmers University

Coordinating WARA representative: Ola Engkvist, WARA Medicine

Suggested WASP PhD students: Mehrdad Farahani, Arsham Gholamzadeh Khoee, Laura van Weesep

Challenges to investigate

- Creating agents for performing common tasks in drug discovery
- Connecting agents into a multi-agent system
- Measuring accuracy and analysing failures of a multi-agent system
- Connecting an agent to AstraZeneca's Reinvent tool
- Connecting an agent to suitable cheminformatics tools for assessment of molecule candidates

Resources

The primary computational resources should be HPC clusters for academic use.
WARA-OSP LLM on-demand services

Deliverables

- Agents for common drug discovery tasks

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References

1. McNaughton et al. CACTUS: Chemistry Agent Connecting Tool Usage to Science *ACS Omega* 2024 *9* (46), 46563-46573
2. Bran et al. Augmenting Large Language Models with Chemistry Tools. *Nature Machine Intel.* 2024, 6, 525-535

Keywords

Drug discovery, tool agents, multi-agent systems, large language models