Abstract

The increasing complexity of environmental and analytical processes in the fields of biology and chemistry requires innovative digital support systems. This project aims to develop a multi-agent system (MAS) that supports researchers through intelligent task sharing, data-driven analyses and knowledge retrieval.

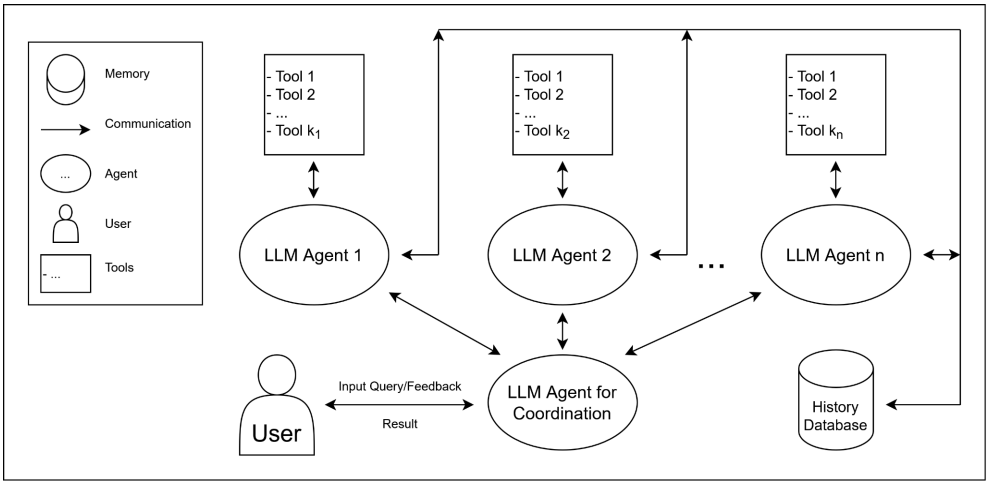
At the centre of the system is a coordinator agent that acts as the central control unit. It analyses incoming requests, decomposes them into manageable subtasks, and assigns them to specialised agents. Each specialised agent is designed for a specific function, such as data analysis, mathematical computation, chemical structure recognition, or knowledge extraction. These agents register their expertise with the coordinator, enabling it to efficiently distribute tasks. The results of each agent's computations are iteratively sent back to the coordinator, which consolidates them and determines if further processing is required before delivering a final response to the user.

The agents are powered by Large Language Models (LLMs), which serve as their reasoning and communication backbone. Additionally, the agents have tool-calling capabilities, allowing them to interact with external environments, perform complex calculations, and retrieve relevant scientific data. These tools include database access for structured information retrieval, API-based knowledge extraction, web queries for real-time data acquisition, and even neural networks that provide supplementary computational capabilities. The system also incorporates a Retrieval-Augmented Generation (RAG) framework, which enables the agents to query domain-specific knowledge bases, scientific literature, and experimental results, thereby ensuring that responses remain contextually accurate and up to date.

A key component of the system is the Human-in-the-Loop (HITL) mechanism, which allows users to provide continuous feedback. By reviewing and correcting outputs, human experts refine the system's accuracy and efficiency, fostering a self-improving cycle of learning. Over time, this feedback-driven adaptation enhances the MAS's ability to handle increasingly complex scientific inquiries.

The project represents a new type of adaptive and collaborative architecture for use in scientific laboratories. Potential use cases include TLC (thin-layer chromatography), tumour research, and battery recycling. This approach is intended to increase the efficiency and precision of scientific processes and create an interactive research assistant.

By leveraging multi-agent collaboration, advanced AI models, and human oversight, this project aims to create an adaptive and intelligent system that significantly improves the efficiency and precision of scientific processes in biology and chemistry.



The diagram illustrates the architecture of the proposed Multi-Agent System (MAS), which integrates Large Language Models (LLMs), specialized tools, and a coordination mechanism to support laboratory work.

1. User Interaction:
    - The user initiates a query or task request, which is processed by the LLM Agent for Coordination.
    - Users can also provide feedback to improve the system's accuracy and efficiency.
2. LLM Agent for Coordination:
    - This central agent decomposes complex queries into subtasks and assigns them to specialized LLM agents.
    - It consolidates results from different agents and, if necessary, initiates further processing before delivering a final result to the user.
3. Specialized LLM Agents:
    - Each LLM Agent is designed for a specific task and has access to domain-specific tools (e.g., chemical analysis tools, database queries, mathematical computations, image processing, robot control).
    - The agents can interact with external tools to retrieve scientific data, perform calculations, or access structured knowledge bases.
    - Each agent registers its expertise with the coordinator, enabling efficient task distribution.
4. Memory and Knowledge Retrieval:
    - The system integrates a History Database, allowing agents to store and retrieve past interactions and results.
    - Additionally, a Retrieval-Augmented Generation (RAG) framework provides access to external scientific literature, experimental data, and structured databases, ensuring contextually accurate and up-to-date responses.
5. Feedback and Adaptation:
    - The Human-in-the-Loop approach allows users to correct and refine the system’s responses, leading to continuous learning and improvement.

This MAS architecture ensures efficient collaboration between multiple intelligent agents, enabling automated reasoning, data analysis, and real-time knowledge retrieval in scientific research.