AI-Driven Workflow Planning for Robotic Arms in Self-Driving Labs

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Introduction

Self-driving labs (SDLs) combine hardware and software to automate the planning and execution of experiments. However, programming workflows to operate robotic arms is time-consuming and error-prone. How can we provide an **accessible** way for chemists to rapidly generate code to **safely** operate **robotic arms** in SDLs?

Challenge	There is a **disconnect** between a chemical procedure and the robotic movements.[1]
Solution	**Large Language Models** (LLMs) can generate experimental workflows for SDLs.[2]
Challenge	LLMs **hallucinate** and cannot reason, so they may not generate code that **safely** operates robotic arms.
Solution	Use **formal reasoning**[3] to generate safe workflows with **classical planners.**[4]

Workflow Overview

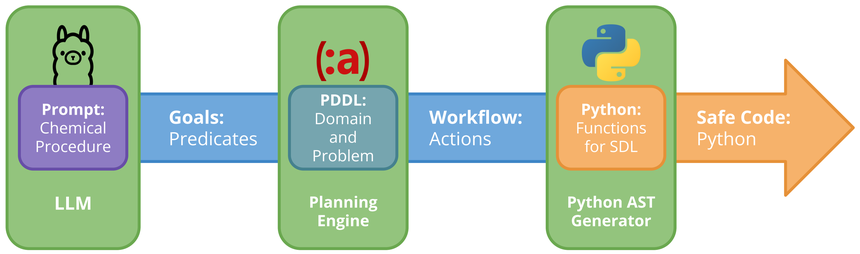

Fig 1. High Level Overview of Program (LLM, Planning Engine, Python Abstract Syntax Tree (AST) Generator)

Results and Future Work

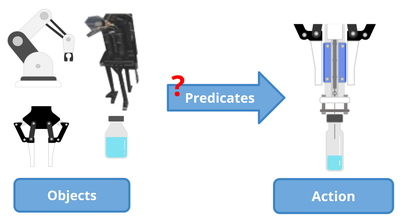

Fig 2. Predicates, or invariants, allow the planner to generate actions that use objects

Simple workflows involving liquid transfer for equipment operation can be reliably generated from natural language.

Future work includes releasing the code as an open-source library and making it easier to add invariants. Finding invariants for the interaction of each piece of equipment with the robotic arm can be a tedious process which could be assisted with another LLM or graphical user interface.

Methods

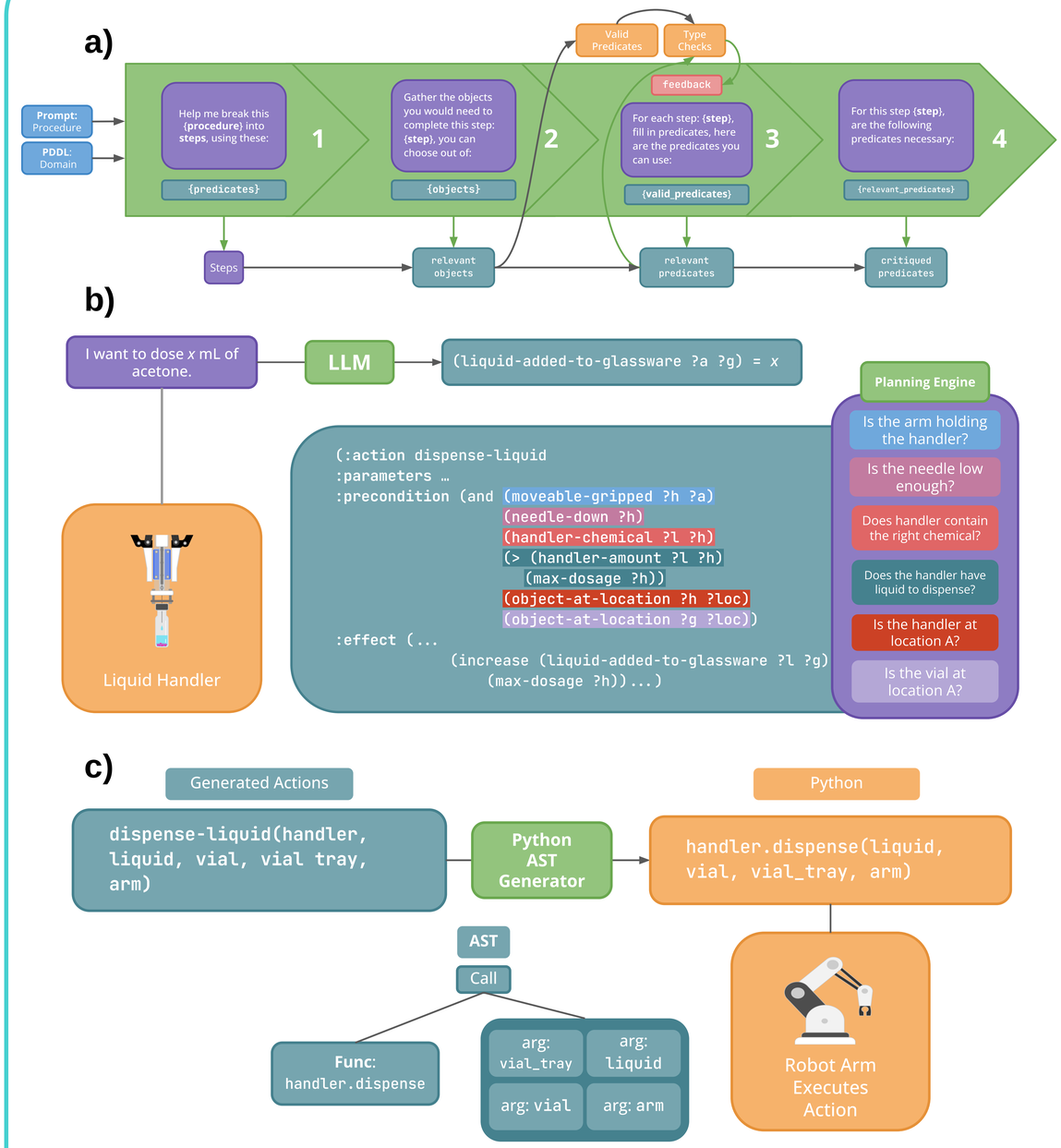

Fig 3. **a)** Prompt pipeline for LLM. **b)** Example of a predicate, and an action that changes the value of that predicate. Questions are presented with each precondition predicate. **c)** High level PDDL actions are mapped to low-level robotic arm and chemical equipment APIs in Python.

1. Christensen, M., et al., (2021). Automation isn't automatic. Chemical Science, 12(47), 15473–15490.
2. Yoshikawa, N., et al., (2023). Large language models for chemistry robotics. Autonomous Robots, 47(8), 1057–1086.
3. Liu, B., et al., (2023, April 22). LLM+P: Empowering Large Language Models with Optimal Planning Proficiency. arXiv.org.
4. Unified Planning: A Python library making planning technology accessible - ICAPS 2023. (n.d.).

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