CLAIRify

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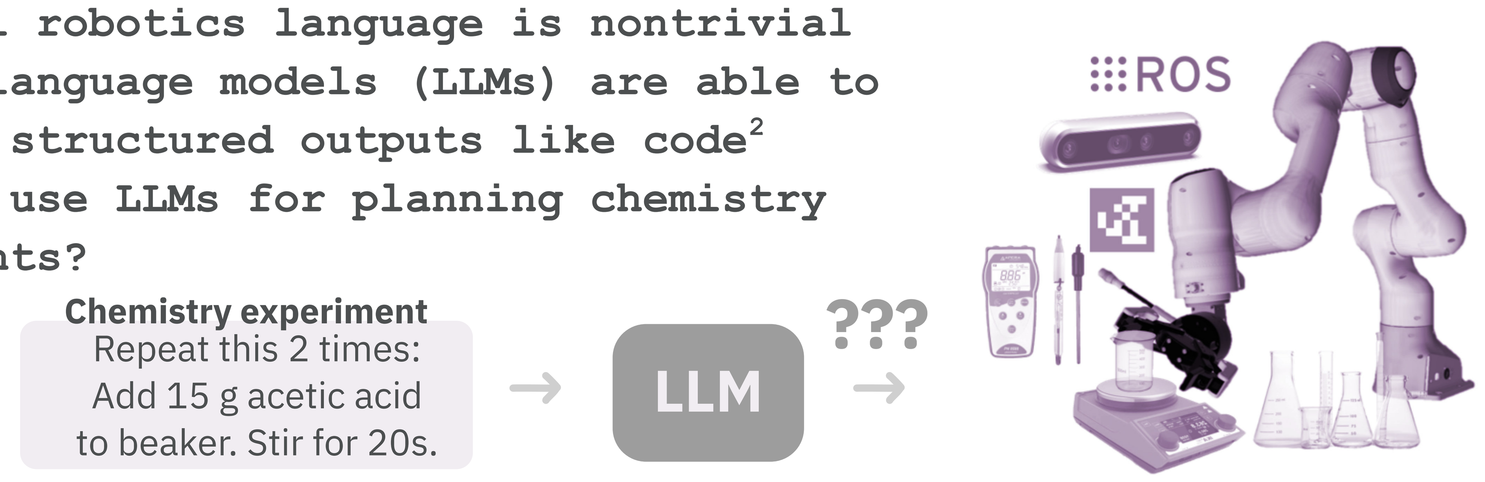
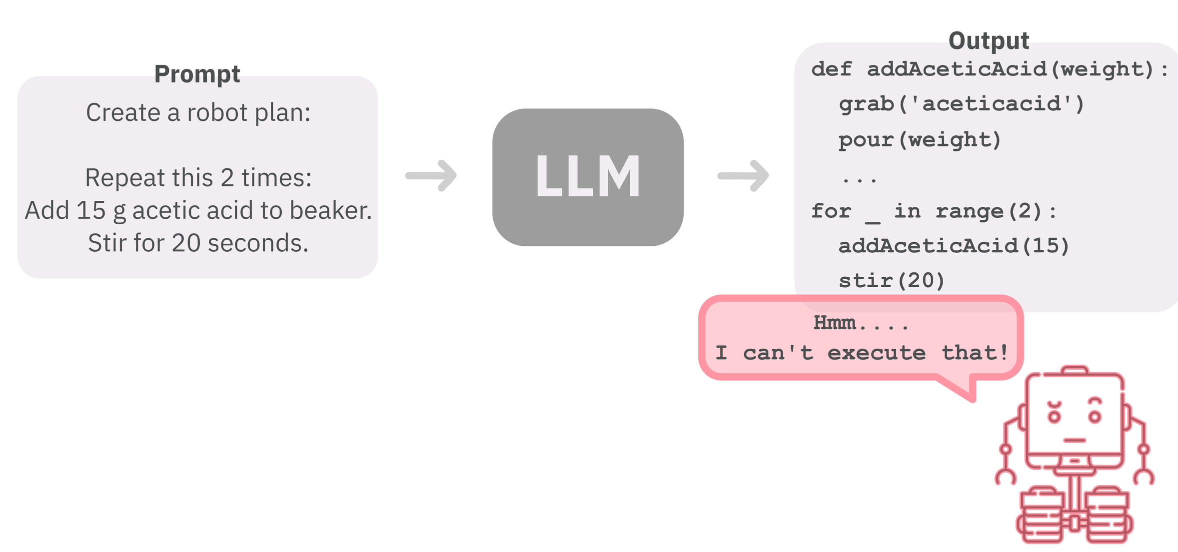
Robotics for Chemistry

- Self-driving labs can accelerate molecular discovery[1]
- Translating experiments from natural language to low level robotics language is nontrivial
- Large language models (LLMs) are able to generate structured outputs like code[2]
- Can we use LLMs for planning chemistry experiments?

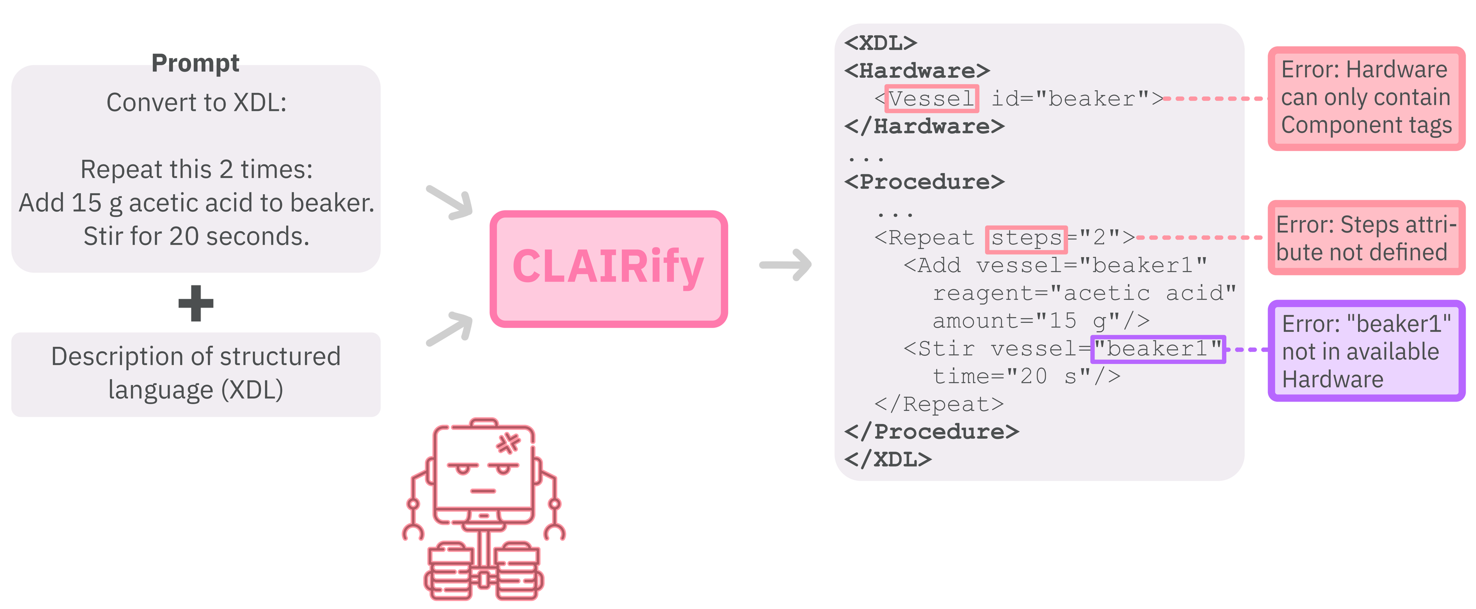


Problems with using LLMs for task plan generation

[1] Poor performance for data-scarce domain-specific languages (DSLs) --> for XDL, a language used in robotics for chemistry lab automation, vanilla zero-shot prompting of LLMs produces erroneous task plans.

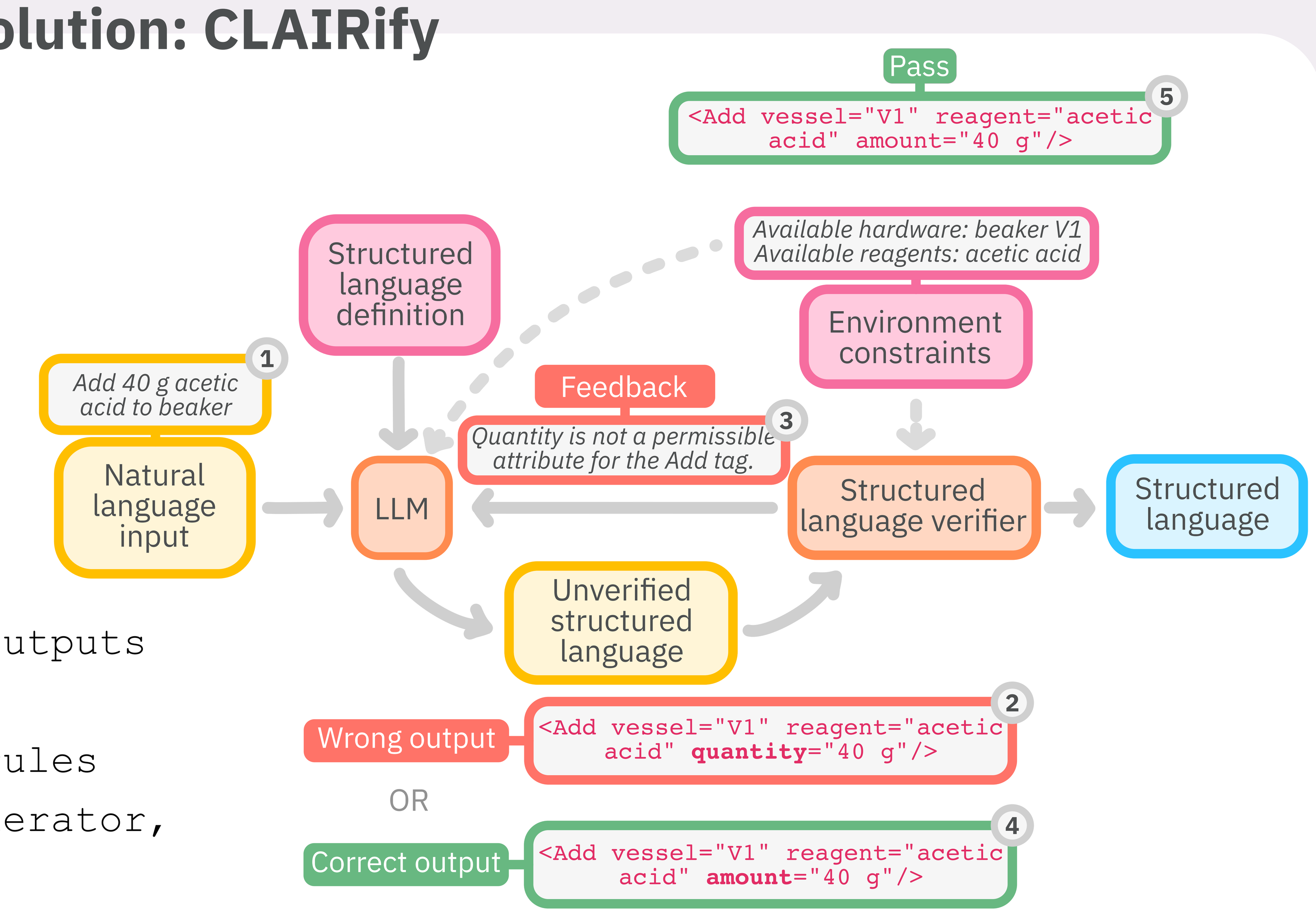


[2] Lack of task plan verification --> generated task plans might be syntactically incorrect and/or incorporate resources not present in the environment.

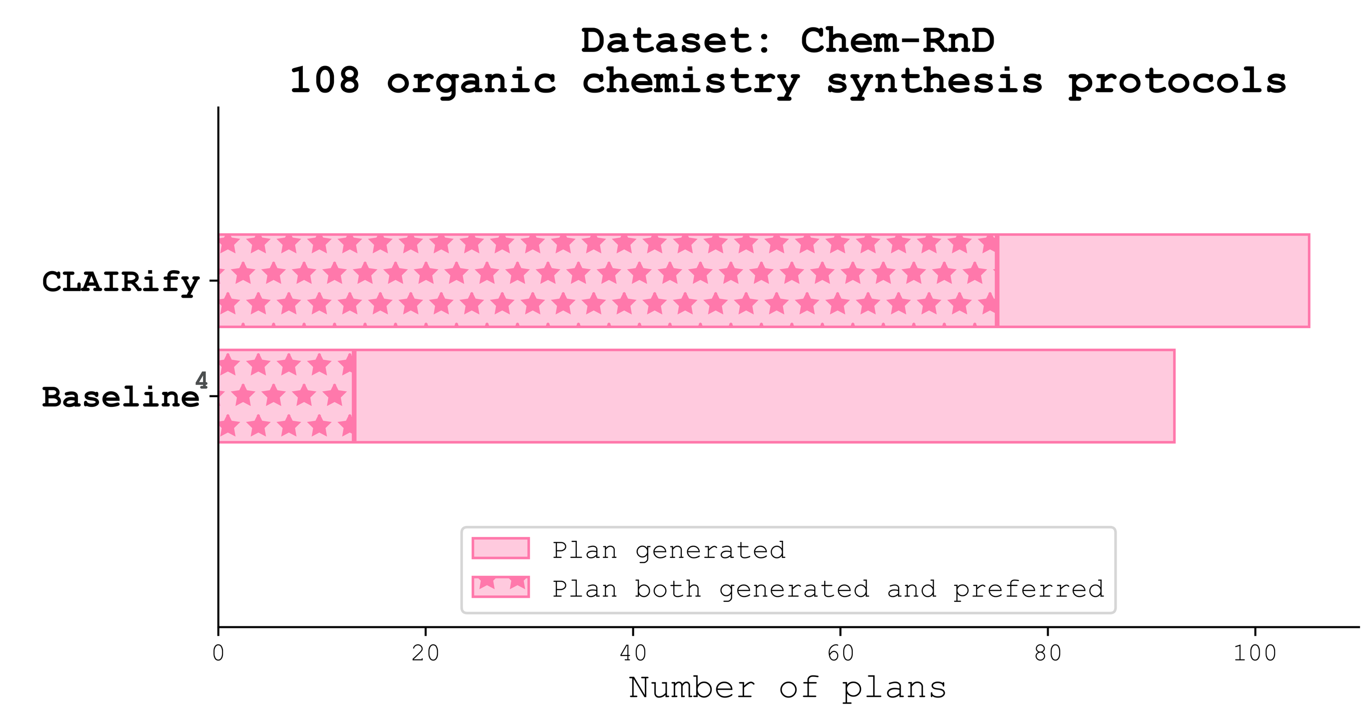


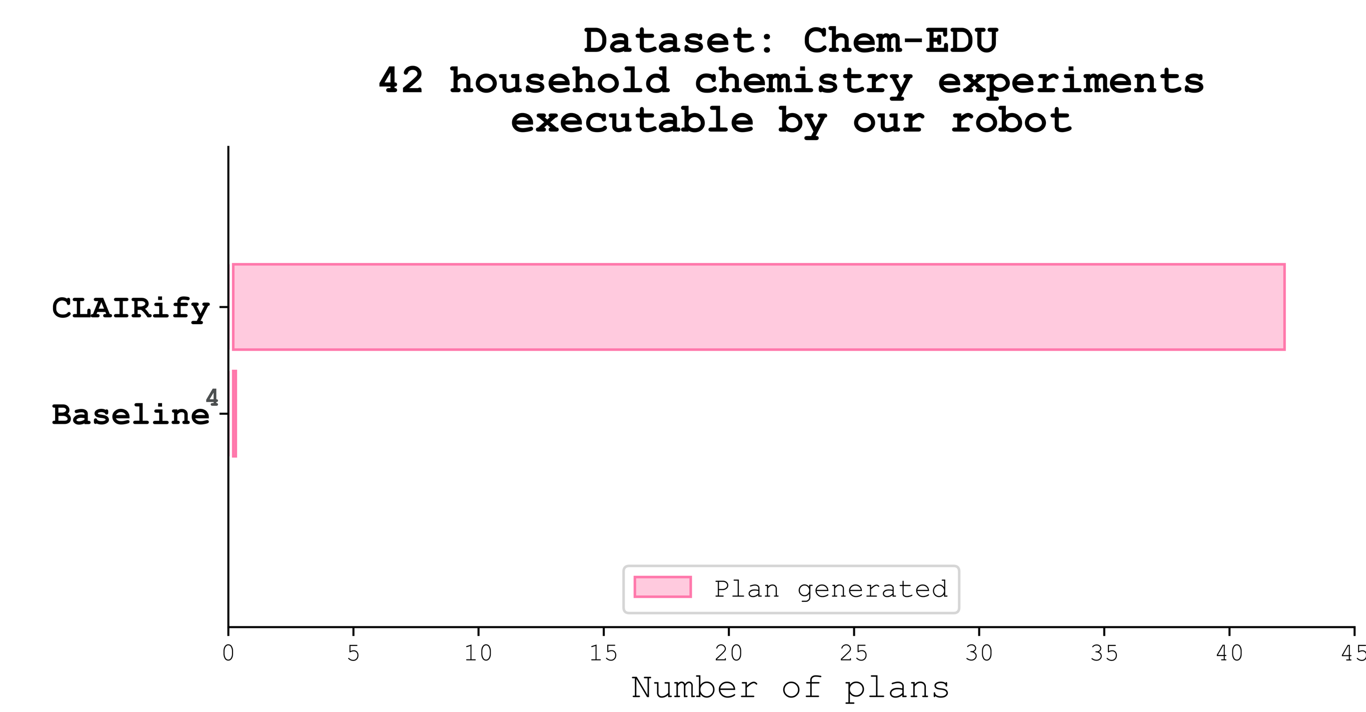
Our solution: CLAIRify

- CLAIRify is a **framework** that translates natural language into a domain-specific structured task plan using an **automated iterative verification** technique to ensure the plan is syntactically valid in the target DSL. It also **takes into account environment constraints** if provided.
- It consists of two parts:
  - [1] **Generator** which takes in DSL rules & natural language instruction, and outputs unverified structured language
  - [2] **Verifier** which checks whether DSL rules are followed; returns feedback to Generator, which re-generates task plan
- To map the plan to robot actions, we use a **Task and Motion Planner**[3]

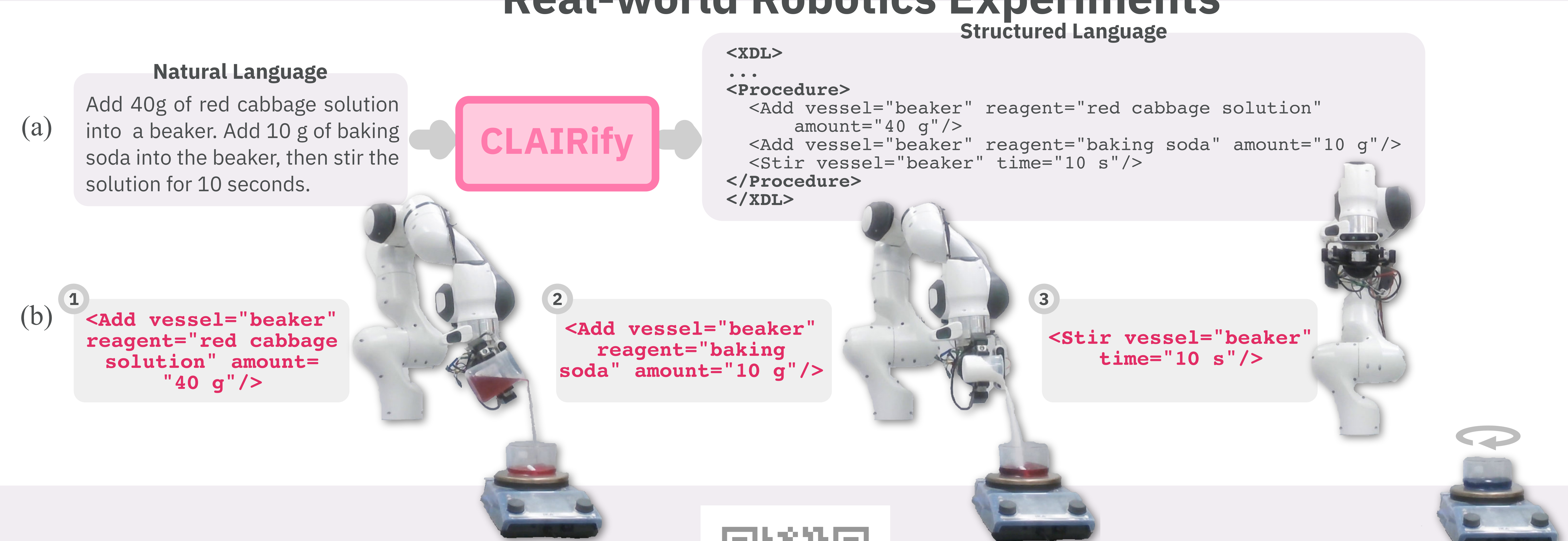


Experiments & Results





Real-world Robotics Experiments



References

[1] M. Seifrid, et al., Autonomous chemical experiments: Challenges and perspectives on establishing a self-driving lab. Acc. Chem. Res., 2022.
[2] I. Singh, et al., "Progprompt: Generating situated robot task plans using large language models," in IEEE Int. Conf. Robot. Autom., 2023.
[3] N. Yoshikawa, et al., "An adaptive robotics framework for chemistry lab automation," arXiv:2212.09672, 2022.
[4] S. H. M. Mehr, et al., "A universal system for digitization and automatic execution of the chemical synthesis literature," Science, vol. 370, no. 6512, pp. 101-108, 2020.

OUR WEBSITE https://ac-rad.github.io/clairify/

ARXiV PAPER https://arxiv.org/pdf/2303.14100

DEMO https://clairify.matter.toronto.edu/moml2023/