Large Language Models for Chemistry Robotics

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Abstract

This paper proposes an approach to automate chemistry experiments using robots by translating natural language instructions into robot-executable plans, using large language models together with task and motion planning. While recent advances have utilized large language models to generate task plans, the issue of executability with embodied agents remains unresolved. To enable autonomous chemistry experiments and alleviate the workload of chemists, robots must interpret natural language commands, perceive the workspace, autonomously plan multi-step actions and motions, consider safety precautions, and interact with various laboratory equipment. Our approach, CLAIRIFY, combines automatic iterative prompting with program verification to ensure syntactically valid programs in a data-scarce domain-specific language that incorporates environmental constraints. The generated plan is executed through solving a constrained task and motion planning (TAMP) problem using PDDLStream solvers to prevent spillages of liquids as well as collisions in chemistry labs. We demonstrate the effectiveness of our approach in planning chemistry experiments, with plans successfully executed on a real robot using a repertoire of robot skills and lab tools. Specifically, we showcase the utility of our framework in pouring skills for various materials and two fundamental chemical experiments for materials synthesis: solubility and recrystallization. Further details about CLAIRIFY can be found at https://ac-rad.github.io/clairify/.

Keywords: Large language models, Constrained task and motion planning, Plan generation verification, Self-driving labs, Chemistry lab automation

1 Introduction

The execution of chemistry experiments, which represents a crucial stage in the process of material discovery, typically relies on human experts. However, manual experimentation poses a number of significant challenges, such as difficulties in reproducibility, high resource requirements, and limited

scalability. To address these obstacles, the concept of self-driving labs (SDLs) has emerged (Seifrid et al., 2022). In order to facilitate access to SDLs by chemists worldwide, it is necessary to enable general-purpose robots to perform a wide range of chemistry tasks and experiments safely and flexibly.

One of the principal obstacles in effectively employing robots in chemistry labs is to ensure that they are natural and intuitive for chemists to operate. An approach to achieving a natural and intuitive interface between chemists and robots is through the use of natural language as a communication medium. This approach enables users to instruct robots in an efficient and effective manner.

This work aims to facilitate autonomous and safe execution of chemistry experiments using general-purpose robot manipulators. This is accomplished through the utilization of natural language instructions to generate plans. Several challenges must be addressed at both the natural language processing (NLP) and robotic planning levels for this purpose. At the NLP level, the robot must be capable of converting natural language instructions into executable robot instructions. At the robotic planning level, the robotic system should be capable of planning robot tasks and motions while taking safety considerations into account, using intermediate goals identified by NLP and perceptual information of the robot workspace.

Natural language has been used in the literature to can overcome the communication barrier between humans and robots, for example in navigation tasks (Tellex et al., 2011). More recently, numerous studies have demonstrated that large language models (LLMs) can assist robots to reason with common sense (Brown et al., 2020; Singh et al., 2022). LLMs have been used to generate structured outputs (Devlin et al., 2019; Brown et al., 2020; Chowdhery et al., 2022), including code generation (Chen et al., 2021; Wang et al., 2021; Li et al., 2022) and robot programming (Liang et al., 2022). Nevertheless, the application of LLMs to task-plan generation for chemistry robots presents two key challenges. First, generated plans must adhere to strict machine-executable syntax rules and be capable of being

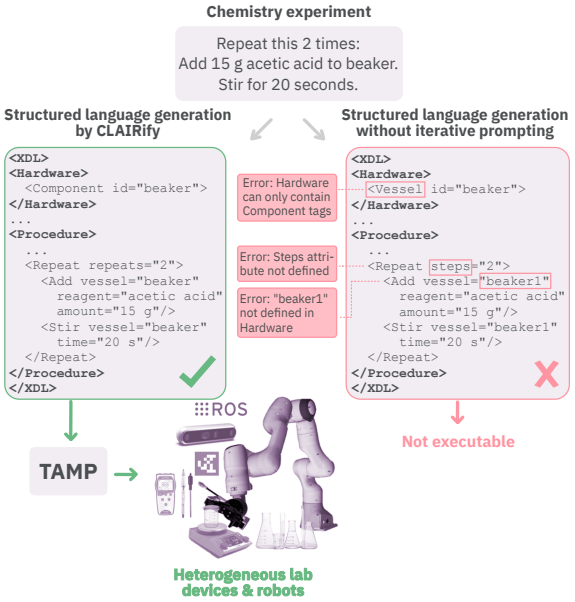


Fig. 1: Task plans generated by LLMs may contain syntactical errors in domain-specific languages. By using verifier-assited iterative prompting, CLAIRIFY can generate a valid program. Once the program has been verified, it is passed on to a task and motion planner (TAMP) for execution by a robot.

executed by the robot, requiring task-plan verification (Garrett et al., 2020; Ahn et al., 2022). Second, LLMs may perform poorly in generating task plans in a zero-shot manner for data-scarce domain-specific languages, such as chemistry (Gu et al., 2021; Liu et al., 2022). Several approaches have been proposed in the literature to address these issues. One promising technique is iterative prompting, which has an advantage over fine-tuning LLMs, as the latter requires large training datasets to learn domain-specific languages reasonably well and incurs high computational costs (Mishra et al., 2021; Wang et al., 2021; Wu et al., 2022). Iterative prompting enables the LLM to verify candidate plans while providing the rules of structured language as input, thereby leveraging the in-context ability of LLMs.

The planning level of the robotic system takes as input perception, vision-based outcome evaluation of experiments and natural language instructions, and solves robot constrained task and motion planning (TAMP) problem. To do

so, robots must possess both general and chemistry domain-specific perception and manipulation skills, including recognizing transparent and opaque objects (Xu et al., 2021; Wang et al., 2023), estimating object poses, and monitoring the state of materials synthesis, for example, detection of a solution when fully dissolved (Shiri et al., 2021). Dexterous manipulation and handling is also necessary, such as constrained motion for picking and transporting objects without spilling their contents, pouring skills, and manipulation of tools and objects. Additionally, high precision and repeatability are crucial for reproducible and reliable results in robot-executed chemistry experiments.

Ensuring safety during experiments and interactions is another challenge (Ménard and Trant, 2020). Multi-layered safety requirements are necessary, including high-level constraints on material synthesis order in experiment description and task planning, and low-level manipulation and perception skills to prevent spilling during transportation of chemistry vials and beakers.

Contributions- We introduce an autonomous robotic system for chemistry lab automation, an end-to-end closed-loop robotic framework that translates natural language into structured long-horizon task plans and then executes them by a constrained task and motion planning solver, integrated with perception and manipulation skills, and vision-based evaluation of experiment outcomes (Figure 1). Our approach consists of two modules. The first is CLAIRify, which translates a natural language input into a structured plan. The second is the translation of the plan to low-level robot actions. To evaluate the framework, we use a domain-specific language called Chemical Description Language (XDL) (Mehr et al., 2020). XDL is an XML-based DSL used to describe action plans for chemistry experiments in a structured format, and is suitable for commanding robots in self-driving laboratories (Seifrid et al., 2022). Our method includes (I) a rule-based iterative verifier to check for syntax correctness and environment constraints, which improves zero-shot task plan generation in a data-scarce domain. (II) At the TAMP level, constrained task and motion planning are incorporated using a PDDLStream (Garrett et al., 2020) solver to avoid spillage when transporting liquids and powders. To improve the success rate of planning, we demonstrate that an 8-DoF robot has 97% success rate compared to 84% of a 7-DoF robot. Moreover, we present accurate and efficient pouring skills inspired by human motions with an average relative error of 8.1% and 8.8% for pouring water and salt, respectively, compared to a baseline method with 81.4% and 24.1% errors. These results are comparable with recent results (Kennedy et al., 2019; Huang et al., 2021), while our method is simpler, and requires fewer and simpler sensors.

Our evaluation results demonstrate that CLAIRify outperforms the current state-of-the-art model for XDL generation presented in (Mehr et al., 2020). Additionally, CLAIR represents a significant advancement from the approach in (Fakhruldeen et al., 2022), which utilized a finite state machine with fixed objects in a static workspace. As a proof of concept for chemistry lab automation, we achieved results that are comparable to the literature ground truth for a *solubility* experiment, with a 7.2% error rate for the solubility of salt, and successful recrystallization of alum.

The paper is organized as follows: Section 2 reviews the state of the art. Section 3 defines the problem and presents the proposed end-to-end approach, covering natural language and perceptual inputs to robot task and motion planning and skill execution. Experiments and results are presented in Section 4. Discussion of the results is provided in Section 5, and conclusions are drawn in Section 6.

2 Related Work

This section describes recent advancements in lab automation, specifically focusing on robotics and the methods through which large language models (LLMs) can be incorporated into these systems. Furthermore, the section highlights the challenges associated with generating verifiable task plans from LLMs, which is necessary to generate robot tasks and motion plans. Lastly, the section outlines recent efforts that focus on identifying the essential robot skills required to execute lab automation tasks effectively.

2.1 Lab Automation

Lab automation aims to introduce automated hardware in a laboratory to improve the efficiency of scientific discovery. An example of lab automation is the usage of mobile robots for improving photocatalysts for hydrogen production from water (Burger et al., 2020). Recently, an automated workflow that translates organic chemistry literature into a structured language called XDL was proposed (Mehr et al., 2020). ARChemist (Fakhruldeen et al., 2022), a lab automation system, was developed to conduct experiments including solubility screening and crystallization without human intervention. Although these major steps towards chemistry lab automation have been made, their dependence on predefined tasks and on motion plans without constraint satisfaction guarantees limits their flexibility in new and dynamic workspaces. In those works, pick & place was the primary task that the manipulators were carrying out. Those works were tested in hand-tuned and static environments to avoid occurrences of unsatisfied task constraints and the associated problems, such as chemical spills during transfer of vessels filled with liquid. Our framework resolves these gaps through using large language models to generate long horizon machine-readable instructions and passing it to a constraint satisfaction and scene-aware planning system with a variety of skills.

2.2 Large Language Models for Chemistry

Several language models specialized for the chemistry or science domain have been proposed, such as MolT5 (Edwards et al., 2022), Chemformer (Irwin et al., 2022), and Galactica (Taylor et al., 2022). After the release of GPT-3, chemistry applications were attempted without further training (Jablonka et al., 2023). The abilities to do Bayesian optimization (Ramos et al., 2023), to use external chemistry tools (Bran et al., 2023), and to synthesize molecules by reading documentation (Boiko et al., 2023) were explored. Our work focuses on increasing the reliability of the output of LLMs without further training by introducing iterative prompting and low-level planning through a task and motion planning framework.

2.3 Leveraging Language Models with External Knowledge

A challenge with LLMs generating code is that the correctness of the code is not assured. There have been many interesting works on combining language models with external tools to improve the reliability of the output. Mind's Eye (Liu et al., 2022) attempts to ground large language model's reasoning with physical simulation. They trained LLM with pairs of language and codes and used the simulation results to prompt an LLM to answer general reasoning questions.

Toolformer (Schick et al., 2023) incorporates API calls into the language model to improve a downstream task, such as question answering, by fine-tuning the model to learn how to call the API. LEVER (Ni et al., 2023) improves LLM prompting for SQL generation by using a model-based verifier trained to verify the generated programs. As SQL is a common language, the language model is expected to understand its grammar. However, for DSLs, it is difficult to acquire training datasets and expensive to execute the plans to verify their correctness. Our method does not require fine-tuning any models or prior knowledge on the target language within the language model. Our idea is perhaps closest to LLM-Augmenter (Peng et al., 2023), which improves LLM outputs by giving it access to external knowledge and automatically revising prompts in natural language question-answering tasks. Our method similarly encodes external knowledge in the structure of the verifier and prompts, but for a structured and formally verifiable domain-specific language. A review on augmenting LLMs with external tools is found in (Mialon et al., 2023).

2.4 Task Planning with Large Language Models

High-level task plans are often generated from a limited set of actions (Garrett et al., 2020), because task planning becomes intractable as the number of actions and time horizon grows (Kaelbling and Lozano-Pérez, 2011). One approach to do task planning is using rule-based methods (Mehr et al., 2020; Baier et al., 2009). More recently, it has been shown that models can learn task plans from input task specifications (Sharma et al., 2021; Mirchandani et al., 2021; Shah et al.,

2021), for example using hierarchical learning (Xu et al., 2018; Huang et al., 2019), regression based planning (Xu et al., 2019), or reinforcement learning (Eysenbach et al., 2019). However, to effectively plan tasks using learning-based techniques, large datasets are required that are hard to collect in many real-world domains.

Recently, many works have used LLMs to translate natural language prompts to robot task plans (Ahn et al., 2022; Huang et al., 2022; Liang et al., 2022; Singh et al., 2022). For example, Inner Monologue (Huang et al., 2022) uses LLMs in conjunction with environment feedback from various perception models and state monitoring. However, because the system has no constraints, it can propose plans that are nonsensical. SayCan (Ahn et al., 2022), on the other hand, grounds task plans generated by LLMs in the real world by providing a set of low-level skills the robot can choose from. A natural way of generating task plans is using code-writing LLMs because they are not open-ended (i.e., they have to generate code in a specific manner in order for it to be executable) and are able to generate policy logic. Several LLMs trained on public code are available, such as Codex (Chen et al., 2021), CodeT5 (Wang et al., 2021), AlphaCode (Li et al., 2022) and CodeRL (Le et al., 2022). LLMs can be prompted in a zero-shot way to generate task plans. For example, Huang et al. (2022) analyzed the planning ability of LLM in virtual environment, Code as Policies (Liang et al., 2022) repurposes code-writing LLMs to write robot policy code, and ProgPrompt (Singh et al., 2022) generates plans that take into account the robot's current state and the task objectives. Text2Motion (Lin et al., 2023) combines LLM with skill feasibility heuristics to guide task planning. Inagaki et al. (2023) generated Python code for an automated liquid-handling robot from natural language instructions. However, these methods generate Pythonic code, which is abundant on the Internet. For domain-specific languages, naive zero-shot prompting is not enough; the prompt has to incorporate information about the target language so that the LLM can produce outputs according to its rules.

Our approach, on the other hand, generates a task plan directly from an LLM in a zero-shot way on a constrained set of tasks which are directly translatable to robot actions. We ensure that the plan is syntactically valid and meets environment constraints using iterative error checking. However, while the generated plan is verified for syntax and constraint satisfaction, it does not consider the robot embodiment and workspace scene, making its execution on a robot uncertified. To address this issue, we integrate the generated task plans as intermediate goals into a certifiable task and motion planner framework, which produces executable trajectories for the robot.

2.5 Task and Motion Planning with Constraints

Task and motion planning (TAMP) simultaneously determines the sequence of high-level symbolic actions, such as picking and placing, and low-level motions for the action, such as trajectory generation. Another TAMP solver, PDDLStream (Garrett et al., 2020), extends PDDL (Aeronautiques et al., 1998), a common language to describe a planning problem mainly targeting discrete actions and states, by introducing streams, a declarative procedure via sampling procedures. PDDLStream reduces a continuous problem to a finite PDDL problem and invokes a classical PDDL solver as a subroutine. Since PDDLStream verifies the feasibility of action execution during planning time, it can inherently enhance safety by avoiding unfeasible plans or plans that may lead to unsafe situations. Nonetheless, PDDLStream does not yet account for constraints in the planning process, for example to avoid material spillage from beakers during transportation, which impedes its deployment in real-world lab environments. For this purpose, sampling-based motion constraint adherence (Berenson et al., 2011) or model-based motion planning (Muchacho et al., 2022) are possible stream choices. To overcome this shortcoming, our work extends PDDLStream with a projection-based sampling technique (Kingston et al., 2019) to provide constraint satisfaction, completeness, and global optimality. The proposed PDDLStream takes intermediate goals generated by LLMs in a structured language as its input.

2.6 Skills and Integration of Chemistry Lab Tools

In the process of lab automation, robots interact with tools and objects within the workspace and require a repertoire of many laboratory skills. Some skills can be completed with existing heterogeneous instruments and sensors in chemistry labs, such as scales, stir plates, pH sensors, and heating instruments. Other skills are currently done either manually by humans in the lab or with expensive special instruments. In a self-driving lab, robots should acquire those skills by effectively using different sensory inputs to compute appropriate robot commands. Pouring is a common skill in chemistry labs. Recent work (Kennedy et al., 2019; Huang et al., 2021) used vision and weight feedback to pour liquid with manipulators. (Kennedy et al., 2019) proposed using optimal trajectory generation combined with system identification and model priors. To achieve milliliter accuracy in water pouring tasks with a variety of vessels at human-like speeds, (Huang et al., 2021) used self-supervised learning from human demonstrations. In this work, we have reached similar results for pouring, using commercial scales that have delayed feedback. Our approach is model-free, and it can pour granular solids as well. Granular solids have different dynamics from liquids, similar to the avalanche phenomenon. Lastly, while executing a chemistry experiment, the robot should possess perception skills to measure progress toward completing the task. For example, in solubility experiments, the robot should perceive when the solution is fully dissolved, and therefore stop pouring the solvent into the solution. There are different ways to measure solubility. In our work, we use the turbidity measure (Shiri et al., 2021), which is based on optical properties of light scattering and absorption by suspended sediment (Kitchener et al., 2017).

3 Methods

We propose an automated robotic experiment platform that takes instructions from a human in natural language and executes the corresponding experiment. The natural language input is converted into a sequence of robot plans written in a structured language by an LLM-based system, CLAIRify. XDL (Steiner et al., 2019) was used as the robot programming language. The task and motion planning module generates the robot motion from the generated XDL. The overview of the proposed method is shown in Figure 2.

3.1 CLAIRify: Natural language to structured programs

CLAIRify takes a chemistry experiment description in natural language and generates a structured experiment plan in XDL format, which will be fed into the subsequent module to generate robot motions. A general overview of the CLAIRify pipeline is given in Figure 2(a).

CLAIRify generates XDL with an automated iterative prompting between a *generator* and a *verifier*. The generator outputs XDL from a prompt that combines the experiment description and the target language format description. However, we cannot guarantee the output from the generator is syntactically valid, meaning that it would definitely fail to compile into lower-level robot actions. To generate syntactically valid programs, we pass the output of the generator through a verifier. The verifier determines whether the generator output follows all the rules and specifications of the target structured language and can be compiled without errors. If it cannot, the verifier returns error messages stating where the errors were found and what they were. These are then appended to the generator output and added to the prompt for the next iteration. This process is repeated until a valid program is obtained, or until the timeout condition is reached. Algorithm 1 describes our proposed method.

Once the generator output passes through the verifier with no errors, we are guaranteed that it is syntactically valid structured language. This output will then be translated into lower-level robot actions by passing it through TAMP for robot execution. Each component of the pipeline is described in more detail below.

3.1.1 Generator

The generator takes a user's instruction and generates unverified structured language using an LLM. The input prompt to the LLM is composed of a description of the target language, a sentence specifying what the LLM should do (i.e. "Convert to XDL"), the command to the LLM,

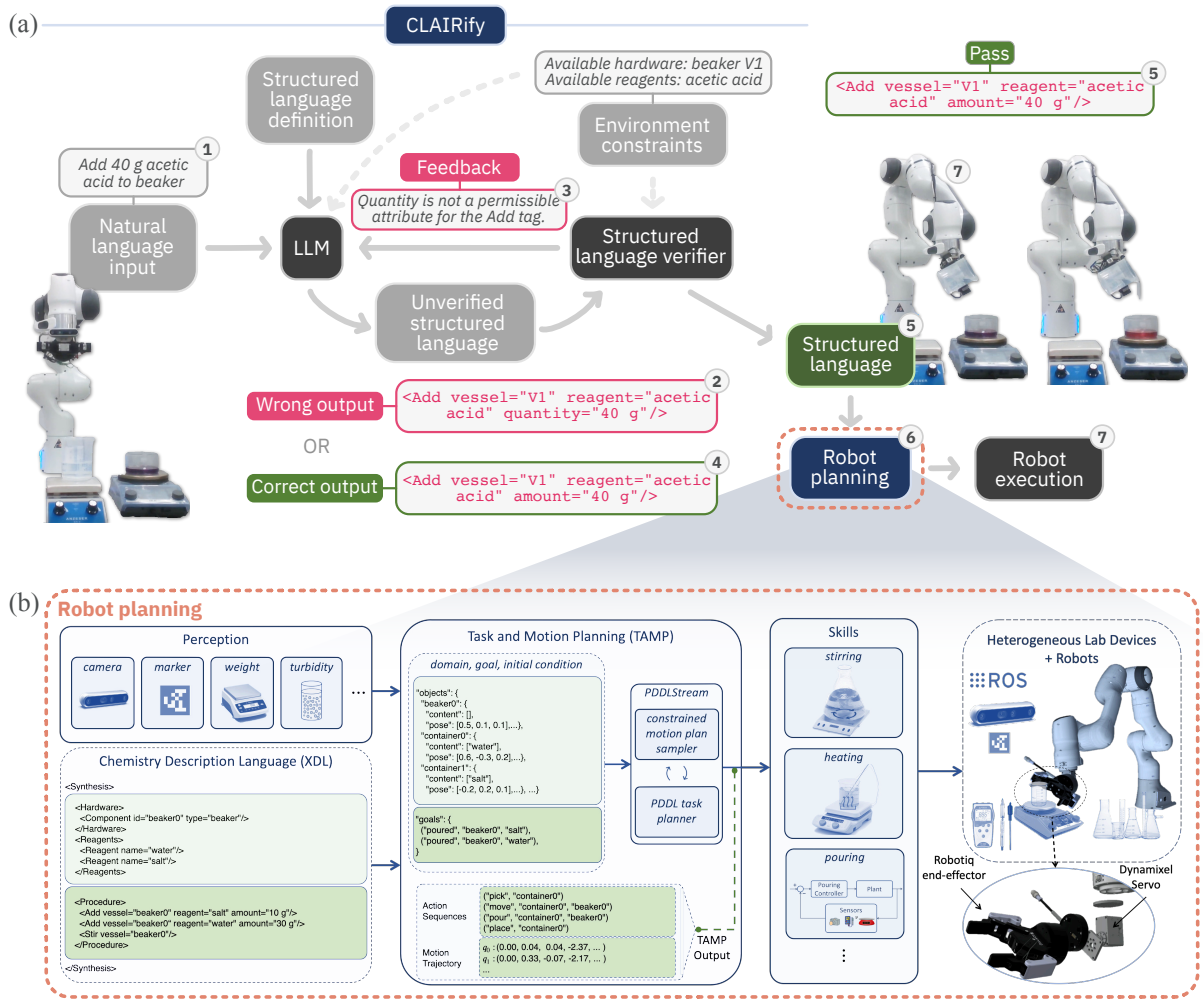


Fig. 2: **Our framework** (a) CLAIRify: LLM-based natural language processing module. The LLM takes the input (1), structured language definition, and (optionally) resource constraints and generates unverified structured language (2). The output is examined by the verifier, and is passed to LLM with feedback (3). The LLM-generated outputs passes through the verifier (4). The correct output (5) is passed to the task and motion planning module (6) to generate robot trajectories. (b) Robot planning module, which is composed of *Perception*, *Task & Motion Planning*, and *Skills* blocks. Our framework enables the robot to leverage available chemistry lab devices (including sensors and actuators) by adding them to the robot network through ROS. The robot is equipped with an additional DoF at the end-effector, allowing it to perform constrained motions. Our framework receives the chemical synthesis goal in XDL format. The *procedure* component is converted into corresponding PDDL goals, and *hardware* and *reagents* components identify the required initial condition for synthesis. *Perception* detects objects and estimates their positions, contents in the workspace, and task progress. PDDLStream generates a sequence of actions for the robot execution (7).

and the natural language instruction for which the task plan should be created. The description of the XDL language includes its file structure and lists of the available actions (can be thought of as functions), their allowed parameters and their documentation. The input prompt skeleton is shown in Snippet 1, Figure 3.

Algorithm 1 CLAIRIFY: Verifier-Assisted Iterative Prompts

Input: Structured language description $\mathcal{L}$, instruction x
Output: Structured language task plan, y_{SL}
  procedure ITERATIVEPROMPTING($\mathcal{L}$, x)
    $y_{SL'}$ = Generator($\mathcal{L}, x$)
    errors = Verifier($y_{SL'}$)
    while len(errors) > 0 and timeout condition != True **do**
      $y_{SL'}$ = Generator($\mathcal{L}, x, y_{SL'}$, errors)
      errors = Verifier($y_{SL'}$)
    end while
    $y_{SL} = y_{SL'}$
  end procedure

Although the description of the target structured language is provided, the output may contain syntactic errors. To ensure syntactical correctness, the generator is iteratively prompted by the automated interaction with the verifier. The generated code is passed through the verifier, and if no errors are generated, then the code is syntactically correct. If errors are generated, we re-prompt the LLM with the incorrect task plan from the previous iteration along with the list of errors indicating why the generated steps were incorrect. The skeleton of the iterative prompt is shown in Snippet 2, Figure 3. The feedback from the verifier is used by the LLM to correct the errors from the previous iteration. This process is continued until the generated code is error-free or a timeout condition is reached, in which case the system reports not being able to generate a task plan.

3.1.2 Verifier

The verifier works as a syntax checker and static analyzer to check the output of the generator and send feedback to the generator. It first checks whether the input can be parsed as correct XML and then checks the allowance of action tags, the existence of mandatory properties, and the correctness of optional properties. This evaluates if the input is syntactically correct XDL. The verifier also checks the existence of definitions of hardware and reagents used in the procedure or provided as environment constraints, which works as a simple static analysis of necessary conditions for executability. If the verifier catches any errors, the candidate task plan is considered to be invalid. In this case, the verifier returns a list of errors it found, which is then fed back to the generator.

```
initial_prompt = """
# <Description of XDL>

# <Hardware constraints(optional)>
# <Reagent constraints (optional)>

Convert to XDL:
# <Natural language instruction>
"""
```

Snippet 1: Initial prompt

```
iterative_prompt = """
# <Description of XDL>

# <Hardware constraints(optional)>
# <Reagent constraints (optional)>

Convert to XDL:
# <Natural language instruction>
# <XDL from previous iteration>
This XDL was not correct.
There were the errors
# <List of errors, one per line>
Please fix the errors
"""
```

Snippet 2: Iterative prompt

Fig. 3: **Prompt skeleton**: (1) At the initial generation, we prompt the LLM with a description of XDL and the natural language instruction. (2) After the LLM generates structured-language-like output, we pass it through our verifier. If there are errors in the generated program, we concatenate the initial prompt with the XDL from the previous iteration and a list of the errors.

3.1.3 Incorporating Environment Constraints

Because resources in a robot workspace are limited, we need to consider those constraints when generating task plans. If specified, we include the available resources into the generator prompt. The verifier also catches if the candidate plan uses any resources aside from those mentioned among the available robot resources. Those errors are included in the generator prompt for the next iteration. If a constraint list is not provided, we assume the robot has access to all resources. In the case of chemistry lab automation, those resources include experiment hardware and reagents.

3.1.4 User Interface

We provide a graphical user interface for CLAIRIFY to increase accessibility. Users can access it via a web browser (Figure 4) and CLAIRIFY

Fig. 4: **Web interface for CLAIRify**. Users input natural language descriptions of the experiment in the left column. XDL is generated in the right column when the user pushes the translate button.

is called by the Python backend implemented in Flask (Grinberg, 2018).

3.2 Task and Motion Planning for Chemistry Experiments

Our task plan execution framework consists of three components: *perception*, *task and motion planning* (TAMP), and a set of manipulation *skills*, as shown in Fig. 2 (b). XDL input coming from CLAIRify provides a high-level description of experiment instructions to the TAMP module. The perception module updates the scene description by detecting the objects and estimating their positions using fiducial markers. We used AprilTag (Olson, 2011). Currently, we assume prior knowledge of vessel contents and sizes, and each vessel is mapped to a unique marker ID. Given the instructions from XDL and the instantiated workspace state information from perception, a sequence of high-level actions and robot trajectories are simultaneously generated by the PDDLStream TAMP solver. The resulting plan is then realized by the manipulation module and robot controller, while closing the loop with perception feedback, such as updated object positions and status of the solution.

The TAMP module converts experiment instructions given by XDL into PDDLStream goals and generates a motion plan. The TAMP algorithm is shown in Alg. 2.

Algorithm 2 TampForLabAutomation()

Input: A XDL recipe χ, sensory input $\mathcal{H}$, PDDLStream domain $\mathcal{D}$
Output: Reference *plan* to execute

$Goals, \mathcal{O} \leftarrow$ xdlParser(χ) ▷ Objects
$\mathcal{I} \leftarrow$ perception($\mathcal{H}, \mathcal{O}$) ▷ Initial conditions
if not passConditions($\mathcal{I}$, $\mathcal{O}$) **then return**
$plan = \emptyset$, $\mathcal{P} = \emptyset$
for all $\mathcal{G} \in Goals$ **do**
  while $time() \leq t_{max}$ **do**
    $\mathcal{P}$ = optimisticPddlStreamPlan($\mathcal{I}$, $\mathcal{G}$, $\mathcal{D}$)
    if $\mathcal{P} \neq \emptyset$ and isStreamFeasible($\mathcal{P}$) **then break**
  end while
  if $\mathcal{P} = \emptyset$ **then return**
  $plan \leftarrow plan \cup \mathcal{P}$
  $\mathcal{I}$ = updateSceneRepresentation($\mathcal{I}, \mathcal{P}$)
end for
return *plan*

3.2.1 PDDLStream

A PDDLStream problem described by a tuple $(\mathcal{P}, \mathcal{A}, \mathcal{S}, \mathcal{O}, \mathcal{I}, \mathcal{G})$ is defined by a set of predicates $\mathcal{P}$, actions $\mathcal{A}$, streams $\mathcal{S}$, initial objects $\mathcal{O}$, an initial state $\mathcal{I}$, and a goal state $\mathcal{G}$. A predicate is a boolean function that describes the logical relationship of objects. A logical action $a \in \mathcal{A}$ has a set of preconditions and effects. The action a can be executed when all the preconditions are satisfied. After execution, the current state changes according to the effects. The set of streams, $\mathcal{S}$, distinguishes a PDDLStream problem from traditional PDDL. Streams are conditional samplers that yield objects that satisfy specific constraints. The goal of PDDLStream planning is to find a sequence of logical actions and a continuous motion trajectory starting from the initial state until all goals are satisfied, ensuring that the returned plan is valid and executable by the robot. We define four types of actions in our PDDLStream domain: *pick*, *move*, *place*, and *pour*. For example, the *move* action translates the robot end-effector from a grasping pose to a placing or pouring pose using constrained motion planning. PDDLStream handles continuous motion using streams. Streams generate objects from continuous variables that satisfy specified conditions, such as feasible grasping pose and collision-free

motion. An instance of a stream has a set of certified predicates that expands $\mathcal{I}$ and functions as preconditions for other actions.

A PDDLStream problem is solved by invoking a classical PDDL planner, such as Fast Downward (Helmert, 2006), with optimistic instantiation of streams (line 7, Alg. 2). If a plan for the PDDL problem is found, the optimistic stream instances $s \in \mathcal{S}$ in the plan are evaluated to determine the actual feasibility (line 8). If no plan was found or the streams are not feasible, other plans are explored with a larger set of optimistic stream instances.

Chemical Description Language (XDL)

XDL is based on XML syntax and is mainly composed of three mandatory sections: `Hardware`, `Reagents`, and `Procedure`. We parse XDL instructions and pass them to the TAMP module. The `Hardware` and `Reagents` sections are parsed as initial objects $\mathcal{O}$. `Procedure` is translated into a set of goals *Goals* (line 1, Alg. 2). $\mathcal{I}$ is generated from $\mathcal{O}$ and sensory inputs (line 2). Each intermediate goal $\mathcal{G} \in \mathit{Goals}$ is processed by PDDLStream (line 5). If a plan to attain $\mathcal{G}$ is found, it is stored (line 10) and $\mathcal{I}$ is updated according to the plan (line 11). After a set of plans to attain all goals is found, we obtain a complete motion plan (line 12).

Plan Refinement at Execution Time

We adopt two considerations for the dynamic nature of chemistry experiments: motion plan refinement and task plan refinement.

The generated motion plan is refined to reflect the updated status of the scene and to overcome the perception errors. The initial object pose detection may contain errors, therefore, the object may not be present in the expected position during execution. This error arises for two reasons. First, when the robot interacts with the objects in the workspace, their position changes, for example when regrasping an object after placing it in the workspace. This change is not always foreseeable by the planner ahead of time. Second, the perception error is lower when the grasping pose is estimated when the robot in-hand camera is closer to the target object, considering the hand-eye calibration error. Lowering the perception error makes the execution more robust to grasping failures. Therefore, to improve the success rate, the object pose is estimated just before grasping, and the trajectory is refined. We assume that the perturbation of the perceived state of the objects is bounded so that it does not cause a change in the logical state of the system, which would necessitate task-level replanning.

In addition to motion refinement, we consider task plan refinement. Task execution can be repeated using the feedback from perception modules at execution time to support conditional operations in chemistry experiments, such as adding acid until pH reaches 7. The number of repetitions required to satisfy conditions is unknown at planning time, so the task plan is refined at execution time.

3.2.2 Motion Constraints for Spillage Prevention

Unlike pick-and-place of solid objects, robots in a chemistry lab need to carry beakers that contain liquids, powders, or granular materials. These chemicals are sometimes harmful, so the robot motion planner should incorporate constraints to prevent spillage. To this end, an important requirement for robot motion is the orientation constraints of the end-effector. To avoid spillage, the end-effector orientation should be kept in a limited range while beakers are grasped. We incorporated constrained motion planning in the framework to meet these safety requirements, under the assumption of velocity and acceleration upper bounds. Moreover, we introduced an additional (8th) degree of freedom to the robot arm, in order to increase the success rate of constrained motion planning. We empirically observed no spillage as long as orientation constraints are satisfied in the regular acceleration and velocity of the robot end-effector, particularly since beakers are typically not filled to their full capacity in a chemistry lab.

Algorithm 3 ConstrainedMotionPlanning()

```
1: for all i ∈ trials do
2:     q_g ← solveIK((^I p_B, ^I R_B))
3:     pathPlanner ← init(q_0, q_g)
4:     while path is ∅ do
5:         q ← sample()
6:         while ‖F(q)‖ > ε do
7:             δq ← J†(q)F(q)
8:             q ← q − δq
9:         end while
10:        path ← pathPlanner(q)
11:    end while
12:    if path ≠ ∅ then return path
13: end for
14: return path
```

Constrained Motion Planning

Given a robot with n degrees of freedom in the workspace $\mathcal{Q} \in \mathbb{R}^n$ with obstacle regions $\mathcal{Q}_{obs} \in \mathbb{R}^n$, the constrained planning problem can be described as finding a path in the manipulator's free configuration space $\mathcal{Q}_{free} = \mathcal{Q} - \mathcal{Q}_{obs}$ that satisfies initial configuration $\boldsymbol{q}_0 \in \mathbb{R}^n$, end-effector goal pose $({}^{\mathcal{I}}\boldsymbol{p}_{\mathcal{B}} \in \mathbb{R}^3, {}^{\mathcal{I}}\boldsymbol{R}_{\mathcal{B}} \in SO(3))$, and equality path constraints $\boldsymbol{\mathcal{F}}(\boldsymbol{q}) : \mathcal{Q} \to \mathbb{R}^k$. The constrained configuration space can be represented by the implicit manifold $\mathcal{M} = \{q \in \mathcal{Q} \mid \boldsymbol{\mathcal{F}}(\boldsymbol{q}) = \boldsymbol{0}\}$. The implicit nature of the manifold prevents planners from directly sampling, since the distribution of valid states is unknown. Further, since the constraint manifold resides in a lower dimension than the configuration space, sampling valid states in the configuration space is highly improbable and thus impractical. Following the constrained motion planning framework developed in (Kingston et al., 2019, 2018), our framework integrates the projection-based method for finding constraint-satisfying configurations during *sampling* as described in Alg. 3. In this work, the constraints are set to the robot end-effector, hence they can be described with geometric forward kinematics, with its *Jacobian* defined as $\boldsymbol{\mathcal{J}}(\boldsymbol{q}) = \frac{\delta \boldsymbol{\mathcal{F}}}{\delta \boldsymbol{q}}$. After sampling from $\mathcal{Q}_{free}$ in line 5, projected configurations $\boldsymbol{q}$ are found by minimizing $\boldsymbol{\mathcal{F}}(\boldsymbol{q})$ iteratively using Newton's method (highlighted in grey). We use probabilistic roadmap methods (PRM*) to plan efficiently in the 8-DoF configuration space found in our chemistry laboratory domain (Karaman and Frazzoli, 2011; Kavraki et al., 1996).

The constrained path planning problem is sensitive to the start and end states of the requested path, since paths between joint states may not be possible under strict or multiple constraints. If constrained planning is executed with any arbitrary valid solution from the IK solver, the planner typically fails. To address this shortcoming, three considerations are made. First, a multi-threaded IK solver with both iterative and random-based techniques is executed, and the solution that minimizes an objective function ϕ is returned with TRAC-IK, proposed in (Beeson and Ames, 2015). During grasping and placing, precision is paramount, and we only seek to minimize the sum-of-squares error between the start and goal Cartesian poses. Second, depending on the robot task, the objective function is extended to maximize the manipulability ellipsoid as described in (Yoshikawa, 1985), which is applied for more complicated maneuvers, such as transferring liquids across the workspace. Finally, note that configuration sampling must account for the fact that multiple goal configurations are possible. For this purpose, Alg. 3 can iterate several times to find various goal configurations in line 2.

8-DoF Robot Arm

To increase the success rate of planning and grasping under non-spillage constraints, we introduced an additional degree of freedom to the 7 DoF Franka robot. The aim of the addition is twofold. First, the 8-DoF robot has a higher empirical success rate in constrained motion planning, which leads to a higher success rate in total task and motion planning. Second, the robot end-effector orientation is changed to flat (parallel to the floor). This usually places the end-effector orientation far from the joint limit, which in turn makes the pouring control easier.

3.2.3 Manipulation and Perception Skills

Chemistry lab skills require a particular suite of sensors, algorithms, and hardware. We provide an interface for instantiating different skill instances through ROS and simultaneously commanding them. For instance, recrystallization experiments in chemistry require both pouring, heating, and

stirring, which uses both weight feedback for volume estimation and skills for interacting with the liquid using available hardware.

Pouring Controller

In chemistry labs, a frequently used skill in chemical experiments is pouring. Pouring involves high intra-class variations depending on the underlying objective (e.g., reaching a desired weight or pH value); the substances and material types being handled (e.g., granular solids or liquids); the glassware being used (e.g., beakers and vials); the overall required precision; and the availability of accurate and fast feedback. Pouring is a closed-loop process, in which feedback should be continuously monitored. Among these pouring actions, in our work we consider the following variations: pouring of liquids and pouring of granular solids. Note that, in contrast to many control problems, pouring is a non-reversible process where we cannot compensate for overshoot (as the poured material cannot go back to the pouring beaker).

Inspired by observations of chemists pouring reagents, we propose a controller that allows the robot to perform different pouring actions. As shown in Fig. 5, the proposed method takes sensor measurements (e.g., weight feedback from the scale) as feedback and a reference pouring target. The algorithm outputs a robot end-effector joint velocity describing oscillations of the arm's wrist. Since sensors are characterized by measurement delays, chemical reactions require time to stabilize, and pouring is a non-reversible action, chemists tend to conservatively pour a small amount of content from the pouring vessel into the target vessel. They periodically wait for some time to observe any effects and then pour micro-amounts again. In our approach, we use a shaping function $s(t)$ to guide the direction and frequency of this oscillatory pouring behavior, while a PD controller lowers the pouring error. The end-effector velocity vector is computed by blending the shaping function $s(t)$ over the PD control signal, $\boldsymbol{v}_{\mathrm{PD}}(t) = \boldsymbol{k}_p e + \boldsymbol{k}_d \dot{e}$, where $e(t) = x_{ref} - x_{fb}$. Fig. 6 shows an example of the angular velocity of the end-effector and the error during actual pouring. More information about the pouring skill method can be found in Appendix .1.

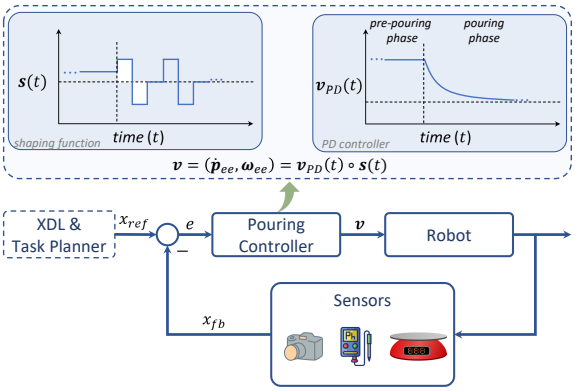


Fig. 5: **Pouring skill controller**: given the XDL & TAMP reference values and sensor feedback, the pouring controller computes the end-effector velocity for the robot by blending a shaping function $\boldsymbol{s}(t)$ and a PD control output $\boldsymbol{v}_{PD}(t)$.

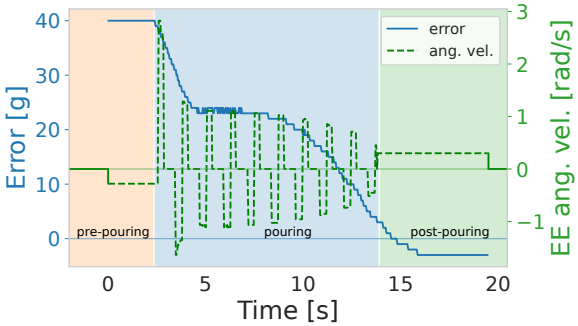


Fig. 6: **An example of pouring control.** The velocity of the end-effector is controlled based on the feedback error and shaping function.

Turbidity-based Solubility Measurement

Solubility of a solute is measured by determining the minimum amount of solvent (water) required to dissolve all solutes at a given temperature when the overall system is in equilibrium (Shiri et al., 2021). Since the solutions get transparent when all solutes dissolve into water, turbidity, or opaqueness of the solution, is used as the metric to determine the completion of the experiment. The average brightness of the solution was used as a proxy for the relative turbidity, inspired by HeinSight (Shiri et al., 2021). That work compared the current measured turbidity value with a reference value (coming from pure solvent) to determine when the solute was dissolved. Differently from them, we use the relative turbidity

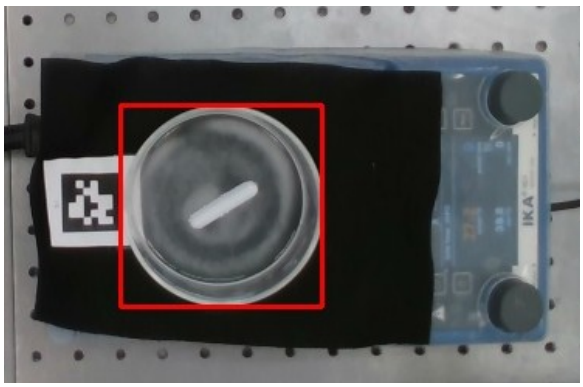


Fig. 7: An example of automated turbidity measurement. The camera detects the Petri dish using Hough Circle Transform. The average brightness of the detected area (red square) is used as a proxy of turbidity.

changes between the current and previous measurement values to detect when the solution is dissolved. Moreover, to make the perception pipeline autonomous, when the robot with an in-hand camera observes the dish containing the solution, it detects the largest circular shape as the dish using a Hough Circle Transform implemented in OpenCV. The square region containing the dish is converted into the HSV color space, and the average Value (brightness) of the region is used as a turbidity value. Figure 7 shows an example of the automated turbidity measurement. Although the detected area contains the dish and stir bar, they do not affect the relative value because these are a constant bias in all measurements.

4 Experiments

4.1 XDL Generation

We conducted experiments to evaluate the following hypotheses: i) Automated iterative prompting increases the success rate of unfamiliar language generation, ii) The quality of generated task plans is better than existing methods. To generate XDL plans, we use `text-davinci-003`, the most capable GPT-3 model at the time of writing. We chose to use this instead of `code-davinci-002` due to query and token limits.

4.1.1 Datasets

We evaluated our method on two different datasets:

Chem-RnD [Chemistry Research & Development]

This dataset consists of 108 detailed chemistry-protocols for synthesizing different organic compounds in real-world chemistry labs, sourced from the Organic Syntheses dataset (volume 77) (Mehr et al., 2020). Due to GPT-3 token limits, we only use experiments with less than 1000 characters. We use Chem-RnD as a proof-of-concept that our method can generate task plans for complex chemistry methods. We do not aim to execute the plans in the real world, and so we do not include any constraints.

Chem-EDU [Everyday Educational Chemistry]

We evaluate the integration of CLAIRify with real-world robots through a dataset of 42 natural language instructions containing only safe (edible) chemicals and that are, in principle, executable by our robot. The dataset consists of basic chemistry experiments involving edible household chemicals, including acid-base reactions and food preparation procedures[1]. When generating the XDL, we also included environment constraints based on what equipment our robot had access to (for example, our robot only had access to a mixing container called "beaker").

4.1.2 Metrics and Results

The results section is organized based on the four performance metrics that we will consider, namely: Ability to generate structured-language output, Quality of the generated plans, Number of interventions required by the verifier, and Robotic validation capability. We compared the performance of our method with SynthReader, a state-of-the-art XDL generation algorithm which is based on rule-based tagging and grammar parsing of chemical procedures (Mehr et al., 2020).

(1) **Ability to generate a structured language plan.** First, we investigate the success

[1] **CLAIRify Data & code:** https://github.com/ac-rad/xdl-generation/

Table 1: Comparison of our method with existing methods on the number of successfully generated valid XDL plans and their quality on 108 organic chemistry experiments from (Mehr et al., 2020).

Dataset	Method	Number generated ↑	Expert preference ↑
Chem-RnD	SynthReader (Mehr et al., 2020)	92/108	13/108
	CLAIRIFY [ours]	**105/108**	75/108
Chem-EDU	SynthReader (Mehr et al., 2020)	0/42	-
	CLAIRIFY [ours]	**42/42**	-

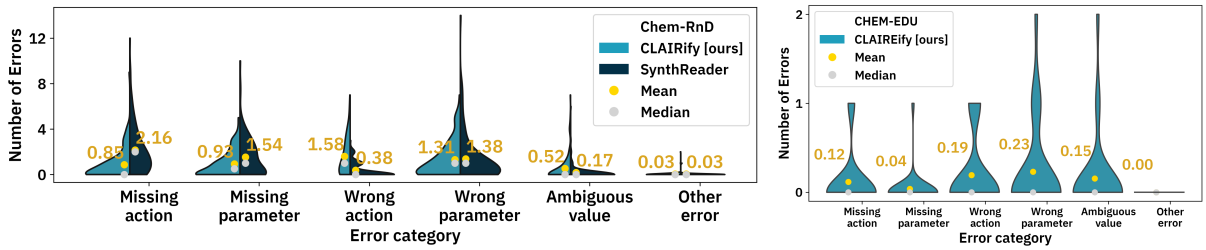


Fig. 8: **Violin plots showing distributions of different error categories in XDL plans generated for experiments for the Chem-RnD (left) and Chem-EDU (right) datasets**. The x-axis shows the error categories and the y-axis shows the number of errors for that category (lower is better). For the Chem-RnD dataset, we show the error distributions for both CLAIRIFY and SynthReader. Each violin is split in two, with the left half showing the number of errors in plans generated from CLAIRIFY (teal) and the right half showing those from SynthReader (navy). For the Chem-EDU dataset, we only show the distributions for CLAIRIFY. In both plots, we show the mean of the distribution with a gold dot (and the number beside in gold) and the median with a grey dot.

probability for generating plans. For CLAIRIFY, if it is in the iteration loop for more than x steps (here, we use $x = 10$), we say that it is unable to generate a plan and we exit the program. When comparing with SynthReader, we consider that approach unable to generate a structured plan if the SynthReader IDE (called ChemIDE[2]) throws a fatal error when asked to create a plan. For both models, we also consider them unable to generate a plan if the generated plan only consists of empty XDL tags (i.e., no experimental protocol). For all experiments, we count the total number of successfully generated language plans divided by the total number of experiments. Using this methodology, we tested the ability of the two models to generate output on both the Chem-RnD and Chem-EDU datasets. The results for both models and both datasets are shown in Table 1. We find that out of 108 Chem-RnD experiments, CLAIRIFY successfully returned a plan 97% of the time, while SynthReader returned a plan 85% of the time. For the Chem-EDU dataset, CLAIRIFY generated a plan for all instructions. SynthReader was unable to generate any plans for that dataset, likely because the procedures are different from typical chemical procedures (they use simple action statements). This demonstrates the generalizability of our method: we can apply it to different language styles and domains and still obtain coherent plans.

(2) **Quality of the predicted plan (without executing the plan)**. To determine if the predicted task plans actually accomplish every step of their original instructions, we report the number of actions and parameters that do not align between the original and generated plan, as annotated by expert experimental chemists. To compare the quality of the generated plans between CLAIRIFY and SynthReader, we ask expert experimental chemists to, given two anonymized plans, either pick a preferred plan among them or classify them as equally good. We also ask them to annotate errors in the plans

[2]ChemIDE using XDL:
https://croningroup.gitlab.io/chemputer/xdlapp/

in the following categories: Missing action, Missing parameter, Wrong action, Wrong parameter, Ambiguous value, Other error. Here, actions refer to high-level steps in the procedure (e.g., `<Add reagent="acetic acid">` is an action) and parameters refer to reagents, hardware, quantities and experiment descriptors (e.g., in `<HeatChill vessel="beaker" temp="100C">`, vessel and temp are both parameters). The annotations were performed using the LightTag Text Annotation Tool (Perry, 2021).

Chem-RnD dataset

The results for the Chem-RnD dataset with respect to expert preference are reported in the last column of Table 1. We found that out of 108 experiments, experts preferred the XDL plan generated from CLAIRify 75 times and the one from SynthReader 13 times (the remaining 20 were considered to be of similar quality).

The distributions of the annotated errors are shown in Figure 8. We find that for 4 out of 6 error categories, our model does at least as well as or better than the baseline method when considering the mean and median of the distributions. We also find that for those categories, our method produces more experiments with 0 errors.

One advantage of our method is that it generates less plans with missing actions compared with the baseline. As XDL generation in SynthReader is implemented by rule-based pattern-matching techniques, any actions that do not match those templates would not appear in the final XDL. For example, for the protocol:

```
To a solution of m-CPBA (200 mg, 0.8 mmol) in
dichloromethane (10 mL), cooled to 0 °C, was
added dropwise a solution of 5-chloro-10-oxa-3-
thia-tricyclo [5.2.1.01, 5] dec-8-ene (150 mg,
0.8 mmol) in dichloromethane (10 mL).
```

the plan generated by CLAIRify was

```
<Add vessel="V1" reagent="m-CPBA" amount="200 mg
"/>
<Add vessel="V1" reagent="dichloromethane"
volume="10 mL"/>
<HeatChill vessel="V1" temp="0 °C" time="3 min"/
>
<Add vessel="V2" reagent="5-chloro-10-oxa-3-thia
-tricyclo[5,2,1,0*1,5*]dec-8-ene" amount="150 mg
"/>
<Add vessel="V2" reagent="dichloromethane"
volume="10 mL"/>
<Transfer from_vessel="V2" to_vessel="V1"/>
```

while the plan generated from SynthReader was

```
<Add vessel="reactor" reagent="5-chloro-10-oxa
-3-thia-tricyclo" volume="0" speed="40.0"/>
```

Our model is able to decompose a complicated procedure into simpler actions by making two solutions in separate beakers and combining them with a Transfer procedure. It also assumes that the solutions don't already exist as mixtures and creates them from scratch. This is another benefit of our model, as it is able to understand implicit actions. For example, given the prompt

```
L-Ornithine (31.92 g, 120 mmol) was added to a
mixture of KOH (6.72 g, 120 mmol), water (200 ml
) and THF (100 ml)
```

SynthReader considers a mixture of three chemicals as a single solution and creates the action:

```
<Add vessel="reactor" reagent="a mixture of KOH
(6.72 g, 120 mmol), water (200 ml) and THF (100
ml)" volume="0" speed="40.0"/>
<AddSolid vessel="reactor" reagent="L-Ornithine"
 mass="31.92 g"/>
```

On the other hand, CLAIRify correctly understand the implicit action to mix them beforehand and generates an appropriate XDL:

```
<Add vessel="V1" reagent="L-Ornithine" amount="
31.92 g"/>
<Add vessel="V1" reagent="KOH" amount="6.72 g"/>
<Add vessel="V1" reagent="Water" amount="200 ml"
/>
<Add vessel="V1" reagent="THF" amount="100 ml"/>
```

However, our model produced plans with a greater number of wrong actions than SynthReader. This is likely because our model is missing domain knowledge on certain actions that would need to be included in the prompt or verifier. For example, given the instruction *"Dry solution over magnesium sulfate"*, our model inserts a `<Dry .../>` into the XDL plan, but the instruction is actually referring to a procedure where one passes the solution through a short cartridge containing magnesium sulphate, a procedure which seems to be encoded in SynthReader. Another wrong action our model performs is reusing vessels. In chemistry, one needs to ensure a vessel is uncontaminated before using it. However, our model generates plans that can use the same vessel in two different steps without washing it in between. Our model also sometimes generates plans with ambiguous values. For example, many experiment descriptions include conditional statements such as "Heat the solution at the boiling point until it becomes white". Conditions in XDL need a numerical condition as a parameter. Our model tries to incorporate them by including actions such as `<HeatChill temp="boiling point" time="until it becomes white"/>`,

Table 2: **Verifier Analysis**. We report the average number of times CLAIRIFY calls the verifier for the experiments in a given dataset, as well as the minimum and maximum number of times. We also report the type of error encountered by the verifier and the number of times it caught that type.

Dataset	Average num. verifier calls	Max/min verifier calls	Error type caught by verifier [count]
Chem-RnD	2.58 ± 2.00	10/1	- missing property in action [306] - property not allowed [174] - wrong tag [120] - action does not exist [21] - item not defined in Hardware or Reagents list [15] - plan cannot be parsed as XML [6]
Chem-EDU	1.14 ± 0.47	3/1	- item not defined in Hardware or Reagents list [47] - property not allowed [26] - wrong tag [40] - missing property in action [3]

but they are ambiguous. We can make our model better in the future by incorporating more domain knowledge into our structured language description and improving our verifier with real-world constraints. For example, we can incorporate visual feedback from the environment, include look-up tables for common boiling points, and ensure vessels are not reused before cleaning.

Despite the XDL plans generated by our method containing errors, we found that the experts placed greater emphasis on missing actions than ambiguous or wrong actions when picking the preferred output, indicating larger severity of this class of error for the tasks and outputs investigated here.

Chem-EDU dataset

We annotated the errors in the Chem-EDU datasets using the same annotation labels as for the Chem-RnD dataset. The breakdown of the errors is in the right plot of Figure 8. Note that we did not perform a comparison with SynthReader as no plans were generated from it. We find that the error breakdown is similar to that from Chem-RnD, where we see amibiguous values in experiments that have conditionals instead of precise values. We also encounter a few wrong parameter errors, where the model does not include units for measurements. This can be fixed in future work by improving the verifier to check for these constraints.

(3) **Number of interventions required by the verifier.** To better understand the interactions between the generator and verifier in CLAIRIFY, we analyzed the number of interactions that occur between the verifier and generator for each dataset to understand the usefulness of the verifier. In Table 2, we show that each experiment in the Chem-RnD dataset runs through the verifier on average 2.6 times, while the Chem-EDU dataset experiments runs through it 1.15 times on average. The difference between the two datasets likely exists because the Chem-EDU experiments are shorter and less complicated. The top Chem-EDU error encountered by the verifier was that an item in the plan was not defined in the Hardware or Reagents list, mainly because we included hardware constraints for this dataset that we needed to match in our plan. In Figure 9, we show a sample loop series between the generator and verifier.

4.2 Robot execution

To analyze how well our system performs in the real world, we execute a few experiments from the Chem-EDU dataset on our robot. Three experiments from the Chem-EDU dataset were selected to be executed.

Table 3: Number of XDL plans successfully generated for different error message designs in the iterative prompting scheme on a validation set from Chem-RnD.

Variations of Iterative Prompt Design using Verifier Error Messages	Plan's generated success rate (%) ↑
Naive: XDL from previous iteration and string "This XDL was not correct. Please fix the errors."	0
Last Error: Error List from verifier from previous iteration	30
All Errors cumulative: Accumulated error List from all previous iterations	50
XDL + Last Error: XDL and Error List from verifier from previous iteration	100

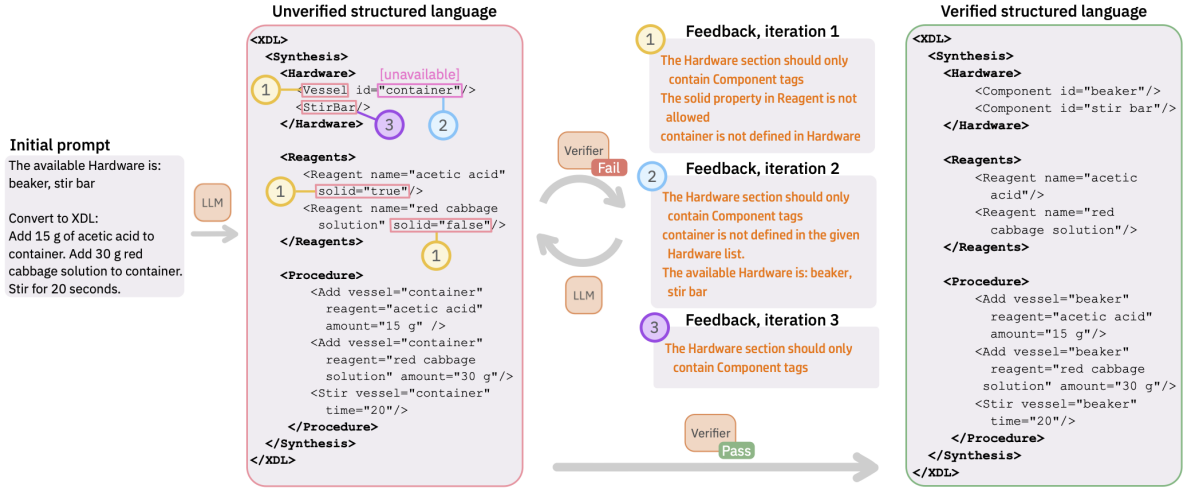


Fig. 9: **Feedback loop between the Generator and Verifier.** The input text is converted to structured-like language via the generator and is then passed through the verifier. The verifier returns a list of errors (marked with a yellow 1). The feedback is passed back to the generator along with the erroneous task plan, generating a new task plan. Now that previous errors were fixed and the tags could be processed, new errors were found (including a constraint error that the plan uses a vessel not in the environment). These errors are denoted with a blue 2. This feedback loop is repeated until no more errors are caught, which in this case required 3 iterations.

4.2.1 Experiment setup

Hardware

The proposed lab automation framework has been evaluated using the Franka Emika Panda arm robot, equipped with a Robotiq 2F-85 gripper and an Intel RealSense D435i stereo camera mounted on the gripper to allow for active vision. The robot's DoF has been extended by one degree (in total 8 DoF) at its end-effector using a Dynamixel XM540-W150 servo motor. Fig. 2 shows the hardware setup.

Lab Tools Integration

The robot framework is expanded by incorporating lab tools. We used an IKA RET control-visc device, which works as a scale, hotplate, and stir plate, and a Sartorius BCA2202-1S Entris, which works as a high-precision weighing scale. The

devices communicate with the TAMP solver to execute chemistry specific skills.

Software

The robot is controlled using FrankaPy (Zhang et al., 2020). We implemented a ROS wrapper for the servo motor (8th DoF). To detect fiducial markers, we use the AprilTag library (Olson, 2011). We use the MoveIt motion planning framework (Coleman et al., 2014) for our TAMP solver and its streams. The constrained planning function (Kingston et al., 2019) is an extension of elion (, 2020).

4.2.2 Solution Color Change Based on pH

As a basic chemistry experiment, we demonstrated the color change of a solution containing red cabbage juice. This is a popular introductory demonstration in chemistry education, as the anthocyanin pigment in red cabbage can be used as a pH indicator (Fortman and Stubbs, 1992). We prepared red cabbage solution by boiling red cabbage leaves in hot water. The colour of the solution is dark purple/red. Red cabbage juice changes its color to bright pink if we add an acid and to blue if we add a base, and so we acquired commercially-available vinegar (acetic acid, an acid) and baking soda (sodium bicarbonate, a base).

In this experiment, we generated XDL plans using CLAIRIFY from two language inputs:

```
[1] Add 40 g of red cabbage solution into a
beaker. Add 10 g of acetic acid into the beaker,
 then stir the solution for 10 seconds.
```

```
[2] Add 40 g of red cabbage solution into a
beaker. Add 10 g of baking soda into the beaker,
 then stir the solution for 10 seconds.
```

Figure 10 shows the flow of the experiment. Our system generated a XDL plan that correctly captured the experiment; the plan was then passed through TAMP to generate a low-level action plan and was then executed by the robot.

4.2.3 Kitchen Chemistry

We then tested whether our robot could execute a plan generated by our model for a different application of household chemistry: food preparation. We generated a plan using CLAIRIFY for the following lemonade beverage, which can be viewed on our website:

```
Add 15 g of lemon juice and sugar mixture to a
cup containing 30 g of sparkling water. Stir
vigorously for 20 sec.
```

4.2.4 Solubility measurement

We finally measured the solubility of household solutes as an example of basic educational chemistry experiments for students (Wolthuis et al., 1960). Measuring solubility has desirable characteristics as a benchmark for automated chemistry experiments: (i) it requires basic chemistry operations, such as pouring, solid dispensing, and observation of the solution status, (ii) solubility can be measured using ubiquitous food-safe materials, such as water, salt, sugar, and (iii) the accuracy of the measurement can be evaluated quantitatively by comparing with literature values. We measured the solubility of three solutes: table salt (sodium chloride), sugar (sucrose), and alum (aluminum potassium sulfate).

The robot estimates the amount of water to make a saturated solution by repeatedly pouring a small amount of water. After pouring, the solution is stirred and the turbidity before and after stirring was compared. The turbidity decreases by stirring if the remaining solutes dissolved into water, whereas it stays at a constant value if there are no residues. If the turbidity decrease after the N-th pouring is smaller than 5%, we assume there were no residues at the beginning of N-th pouring and that the amount of water required to dissolve all solutes is between the volume of water added at the $(N-2)$-th and $(N-1)$-th pouring. We use the average of the two for simplicity of presentation. Figure 12 shows an example of turbidity change during the experiment.

A natural language explanation for the above solubility measurement protocol is as follows:

```
Add 10 g of salt to the beaker.
Repeat the following steps for five times.
Add 10 g of water into the beaker, and measure
the turbidity.
After stirring for 90 seconds, measure the
turbidity again.
```

Note that we extended the XDL to allow turbidity as a measurable quantity of `<Monitor>` since the XDL standard at the time of writing (XDL 2.0.1) only supports temperature and pH. We added this skill to our defintion of XDL that we input to the LLM in CLAIRIFY. The amount of solute and stirring time were changed

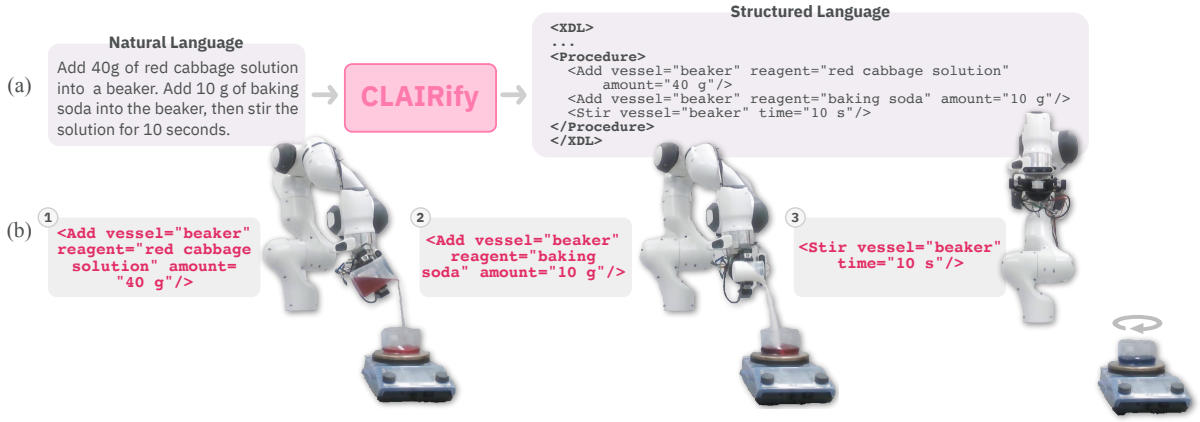


Fig. 10: **Robot execution**: The robot executes the motion plan generated from the XDL for given natural language input. (a) CLAIRIFY converts the natural language input from the user into XDL. (b) The robot interprets XDL and performs the experiment. Stirring is done by a rotating stir bar inside the beaker.

for different solutes. The workflow of the solubility experiments is shown in Fig. 11.

The measured solubility for three solutes is shown in Table 4. The robot framework managed to measure the solubility with sufficient accuracy that they are comparable to solubility values found in the literature (NAOJ, 2022).

Table 4: **Results of the solubility experiments.** Amount of solute in the beaker, amount of water to dissolve all solute, calculated solubility (the amount of solute dissolved per 100 g of water), and literature data for solubility at 20°C is shown. Literature data are taken or calculated from (NAOJ, 2022).

solute	*solute [g]*	*water [g]*	*solubility*	*lit. data*	*% error*
Salt	13.9	41.8	33.2	35.8	7.2
Sugar	60.00	26.46	226.8	203.9	11.2
Alum	3.00	29.87	10.0	11.4	12.3

The primary reason for the difference from the literature value is the range of minimum amount of water required for dissolving. In an example of turbidity change shown in Fig. 12, the robot can only tell the second pouring is insufficient and the third pouring is sufficient to dissolve all solutes, but it cannot tell the exact required amount. As a result, the solubility measurement inherently includes error caused by the resolution of pouring. We can reduce the error by pouring a smaller amount of water at once, but pouring less than 10 g is difficult because of the delayed feedback of the scale and the scale minimum resolution. We can improve the accuracy of solubility measurements by developing a pipette designed for a robot.

4.2.5 Recrystallization Experiment

Recrystallization is a purifying technique to obtain crystals of a solute by using the difference in solubility at different temperatures. Typically, solutes have higher solubility at high temperatures, meaning hot solvents will dissolve more solute than cool solvents. The excess amount of solute that cannot be dissolved anymore while cooling the solvent precipitates and forms crystals. We tested the recrystallization of alum by changing the temperature of the water. Alum was chosen as the target solute since its solubility greatly changes according to water temperature. The recrystallization experiment setup extends the solubility test by pre-heating the solvent. A natural language explanation for the above recrystallization experiment protocol is as follows:

```
Add 50g of water to beaker.
Heat the beaker filled with water for 1 min to
60 C.
Add 20 g of alum into an empty beaker, and add
50 g of the heated water into the beaker.
Cool the beaker for 30 min to 20 C.
```

Fig. 13 shows the result of the experiment.

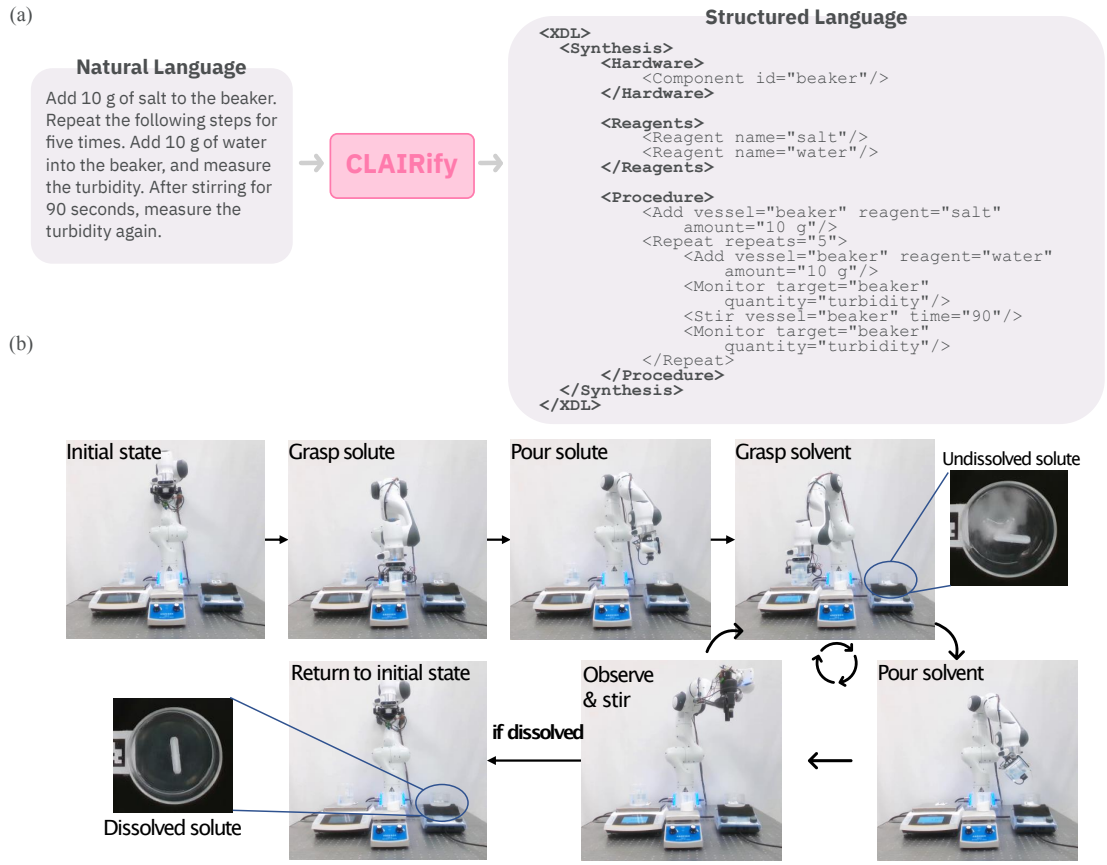


Fig. 11: **Workflow of solubility experiment.** (a) We translate a natural language input to XDL using CLAIRify. (b) We then execute the plan on a robot using TAMP. First, a fixed amount of the solute is added to the dish on the weighing scale and stirrer. The robot pours 10 g of water into the dish. The solution is mixed with the magnetic stirrer. After stirring, the turbidity of the solution is measured to check dissolvement. If undissolved, another 10 g of water is added until no solutes remain. The experiment was conducted at room temperature (25°C).

4.3 Ablation Studies

We assess the impact of various components in our prompt designs and feedback messaging from the verifier. We performed these tests on a small validation set of 10 chemistry experiments from Chem-RnD (not used in the test set) and report the number of XDL plans successfully generated (i.e., was not in the iteration loop for $x = 10$ steps).

4.3.1 Prompt Design

To evaluate the prior knowledge of the GPT-3 on XDL, we first tried prompting the generator without a XDL description, i.e., with the input:

```
initial_prompt = """
Convert to XDL:
# <Natural language instruction>"""
```

The LLM was unable to generate XDL for any of the inputs from the small validation set that contains 10 chemistry experiments. For most experiments, when asked to generated XDL, the model output a rephrased version of the natural language input. In the best case, it output some notion of structure in the form of S-expressions

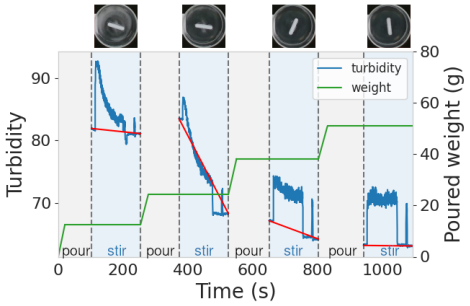


Fig. 12: **Turbidity change during experiment.** Water is poured into the dish during pouring (grey) and turbidity is measured during observation (blue). The end of the experiment is determined by turbidity comparison. In this example, all solutes are dissolved at the third pouring because the turbidity change after the fourth pouring is below the threshold. The average weight of the second and third pouring is used to calculate the solubility.

Fig. 13: **Recrystallization of alum inside the water.** After heating water by putting a beaker with water on a hotplate, the robot poured alum into a dish. The robot then poured hot water, and the solution was heated and stirred. The formation of a precipitate is observed after the dish is cooled down. The dried crystals in a vial are shown.

or XML tags, but the outputs were very far away from correct XDL and were not related to chemistry. We tried the same experiment with `code-davinci-002`; the outputs generally had more structure but were still nonsensical. This result suggests the LLM does not have the knowledge of the target language and including the language description in the prompt is essential to generate an unfamiliar language.

4.3.2 Feedback Design

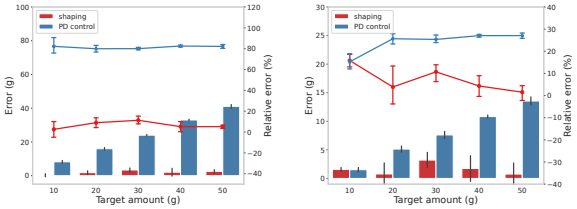
We experimented with prompts in our iterative prompting scheme containing various levels of detail about the errors. The baseline prompt contains a description as well as the natural language instruction. We wanted to investigate how much detail is needed in the error message for the generator to be able to fix the errors in the next iteration. For example, is it sufficient to write "There was an error in the generated XDL", and do we need to include a list of errors from the verifier (such as "Quantity is not a permissible attribute for the Add tag"), or do we also need to include the erroneous XDL from the previous iteration?

We find that including the erroneous XDL from the previous iteration and specifying why it was wrong resulted in the highest number of successfully generated XDL plans. Including a list of errors was better than only writing "This XDL was not correct. Please fix the errors", which was not informative enough to fix any errors. Including the erroneous XDL from the previous iteration is also important; we found that including only a list of the errors without the context of the XDL plan resulted in low success rates.

4.4 Component analysis for robot execution

4.4.1 Pouring Skill Evaluation

We evaluated the accuracy and efficiency of the pouring skill for liquid and powder. To evaluate the effect of our proposed pouring method, we implemented a PD control pouring method where end-effector angular velocity is proportional to the difference between target and feedback weight as a baseline. Fig. 14 shows the pouring experiment results. The results show that the shaping function contributed to reducing the overshooting compared to PD control pouring. The overshoot of the PD control pouring is mainly because of the scale's delayed feedback (∼3 s). The intermittent pouring caused by the shaping function compensated for the delay and improved the overall pouring accuracy. On average the pouring error using the shaping approach is 2.2 ± 1.5 g and for PD control is 24.5 ± 12.0 g and their average relative error and standard deviation are 8.1 ± 4.8 % and 81.4 ± 4.5 %. Moreover, as we can see both the error and relative error stays approximately constant with respect to the target amount when using the shaping method, in contrast to the PD controller. The average pouring time with the shaping function for 50 mL water and salt were 25.1 s and 36.8 s,



(a) Pouring error in water. (b) Pouring error in salt.

Fig. 14: **Evaluation of pouring error**. The pouring errors of our shaping pouring and PD control baseline pouring are compared using (a) water and (b) salt. The bar plot shows the error (poured amount - target amount) and the line plot shows the relative error. The error bars show the standard deviation.

Table 5: **Success rate comparison of 7 and 8-DoF robot.**

	Scenario 1 (%)		*Scenario 2 (%)*	
	IK	***Plan***	***IK***	***Plan***
7 DoF	99	84	99	70
8 DoF	100	97	100	84

respectively. Our results are comparable with previous work (Kennedy et al., 2019; Huang et al., 2021) in terms of pouring error and time, without using a learned, vision-based policy, or expensive equipment setup.

4.4.2 Constrained Motion Planning in 7/8 DoF robot

The constrained motion planning performance of 7 DoF and 8 DoF robot is evaluated in two scenarios: (1) single step, (2) two steps. In scenario (1), robots find a constrained path with a fixed orientation from initial to final positions that are randomly sampled. Scenario (2) extends the first with an additional intermediate sampled waypoint. For each scenario, we run 50 trials in Alg. 3 with random seeding of the IK solver.

In scenario (2), we restart the sequence planning from the first step if a step fails. Constraints are set to the robot end-effector pitch and roll ($\|\theta, \phi\| \leq 0.1$ rad).

The performance of the 7-DoF and 8-DoF robot arms for the two scenarios are shown in Table 5. The results show that the IK and constrained motion planning have higher success rates in 8-DoF compared with the 7-DoF robot.

5 Discussions

In this paper, we demonstrate how LLMs are effective tools for translating natural language inputs into domain-specific target languages without any fine-tuning. We find that by prompting an LLM with errors that it makes, it is able to correct its own output and generate syntactically valid plans. We find that LLMs are robust to variations in natural language, which is important for lowering the barrier to successful user interaction. The XDL plans generated by CLAIRify can then be combined with our TAMP pipeline to effectively perform multistep chemistry experiments in the real world. However, the current study is limited to a few types of chemistry experiments because the number of skills incorporated in the framework is limited. Increasing the repertoire of skills, such as glassware perception in 3D and clutter, without fiducial markers (Eppel et al., 2020), can improve the framework scalability. As we develop more and more skills, we can append their descriptions to the language model input. We demonstrated this by appending a new skill, `<Monitor>`, to the XDL description, and the LLM was able to accurately incorporate it into the plan. Another issue is that the inefficiency of PDDLStream inhibits the framework from being reactive in a dynamic environment. Incorporating the learning-based search heuristics for PDDLStream (Khodeir et al., 2021, 2022) may overcome this limitation. Constrained motion planning was shown to effectively avoid spillage of the beaker contents during transfer in our experiments. We have also shown that adding an extra 8th DoF to the robot enabled more flexibility and a higher success rate for constrained motion planning. However, the proposed constrained motion planning embedded in TAMP cannot run in real-time. Considering the dynamics of the beaker content may help to have higher flexibility in robot manipulation (Muchacho et al., 2022). Although our skill has currently attained 8% error for liquid and powder pouring, higher accuracy is desirable for precise experiments in a chemistry lab. We used a scale with integrated functionality for stirring and heating, but its measurement is delayed for 3 s. Higher precision pouring can be attained using a scale with a shorter response time; also, it can be achieved by specialized tools, such as a pipette. In addition, visual feedback during pouring may avoid spillage.

Moreover, CLAIRify was successful in generating plans beyond the state-of-the-art method for the chemistry domain-specific structured language XDL. Although the generated plans were syntactically correct and satisfied the constraints, they contained errors. However, experts placed greater emphasis on missing actions than on ambiguous or incorrect actions when selecting the preferred output, indicating that this class of error is more severe for the tasks and outputs investigated here. These results demonstrate the generalizability of our method, which uses zero-shot iterative prompting verification. We can apply it to different language styles and domains and still obtain coherent plans. While our approach, which combines LLMs and TAMP, showed promising results in generating feasible and executable plans, as evidenced by our evaluation, the capabilities of pure LLMs in generating semantically correct plans remain limited. The limitation in task planning abilities has been highlighted in a recent study (Bubeck et al., 2023) as well. To address this shortcoming, an alternative approach could be to incorporate human-in-the-loop planning or to utilize multi-modal foundational models that consider the surrounding scene of the robot.

Another important consideration to address is the tradeoff between the human interpretability and expressive power of the target structured language. Our approach to using intermediate language enables users to ensure the LLM's natural language interpretation is reasonable; however, the expressive power of XDL imposed limitations on the framework's abilities. The robot framework can conduct more diverse actions than XDL can express, but the use of XDL limits the available actions. This problem may be alleviated by generating the robot program directly, but human interpretability may be decreased as a result.

6 Conclusions

In this paper, we presented a framework for automating chemistry lab experiments using general-purpose robot manipulators and natural language commands. In order to facilitate the closed-loop execution of long-horizon chemistry experiments, CLAIRify maps natural language commands to XDL, a human-interpretable intermediate language that standardizes chemistry experiment descriptions. Subsequently, XDL instructions are converted into a sequence of subgoals for a constrained task and motion plan solver, and the robot executes those plans using its diverse set of skills. Finally, the robot visually monitors the progress of the tasks. We demonstrated that our approach lowers the barriers to instructing robots by non-experts to execute robot task plans. The robot handles solubility and recrystallization experiments autonomously when provided with natural language inputs.

Declarations

Ethical Statement

Conflict of interest

The authors have no relevant financial or non-financial interest to disclose.

Author Contributions

N.Y., M.S., K.D., S.A.-R., Z.J., L.B.K. worked on CLAIRify; N.Y., K.D., A.Z.L., Y.Z., H.X., A.K. worked on robotic experiments. N.Y., M.S., K.D. wrote the initial draft. L.B.K., A.A.-G., F.S., A.G. proof-read the manuscript, and A.A.-G., F.S., A.G. supervised the project.

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.1 Pouring Policy

The pouring policy is the blending of a shaping function $s(t)$ and a model-free PD controller $\boldsymbol{v}_{\mathrm{PD}}(t)$, expressed as $\boldsymbol{v}_{\mathrm{PD}}(t) \times s(t)$. The PD controller is defined as:

$$\boldsymbol{v}_{\mathrm{PD}}(t) = \boldsymbol{k}_p e + \boldsymbol{k}_d \dot{e}, \tag{1}$$

where $e(t) = x_{ref} - x_{fb}$. The shaping function is implemented via the summation of several unit functions $u(t)$ as follows:

$$\begin{aligned} &s(t) = u(t) - 2\ u(t - t_0) + \\ &\textstyle\sum_{k=1}^{N} \{u(t - (t_0 + k\ T_{deactive})) + \\ &u(t - (t_0 + k\ (T_{deactive} + T_{idle}))) \\ &-2\ u(t - (t_0 + k\ (T_{deactive} + T_{idle} + T_{activate})))\} \end{aligned} \tag{2}$$

where t_0 is the moment in which $e(t)$ starts to change, meaning that the material is getting added to the target dish. $T_{deactive}$, T_{idle}, and T_{active} are the parameters set by the user to describe the periodic motion of the robot end-effector. This motion continues till the material transferred to the target dish reaches the desired amount.