1. Project Description and Program Alignment

Project title: Project title should not exceed 25 words and will be used for Proactive Disclosure and public communication purposes.	
Reinforcement Learning-based Model Predictive Control for Robot Manipulators in Automated Material Design Chemistry Laboratory	
Project description: Project description should not exceed 150 words and may be used for Proactive Disclosure and public communication purposes.	
Automated chemistry for material design has been a priority for research groups and companies per the requirement of increased productivity, reliable results, safer operation conditions, cost savings, and flexible working time. Due to the features of dexterity and flexibility, robot manipulators (RMs) are widely used for chemistry laboratory automation. However, the safe and high-precision control of RMs for pouring and transmitting reagents and catalysts in synthetic and reaction experiments is still challenging. To fill this gap, this project aims to propose a solution to the control of an RM with guaranteed safety, reliability, and stability for achieving autonomous grasping operation. Specifically, the objective of this work is to develop an intelligent framework based on reinforcement learning (RL), model predictive control (MPC), and visual servoing techniques. The proposed RL-based MPC (RLMPC) will improve the control performance of the RM and thus further improve the level of automation in chemistry laboratories.	
Anticipated start date:	September 1st 2023
Anticipated project duration (underline):*	12 months <u>24 months</u>
Master project alignment (underline one):	AI for Biological Systems; AI-Assisted Photonics Design; Deep Material Science; <u>Core AI for Design</u>

* Projects are eligible for extension on a case-by-case basis

Project overview

Briefly describe the scientific opportunity/gap that this project addresses (~150 words)
Material design requires extensive experimentation and testing through an iterative process of evaluation and revision of the produced material to develop an optimal formula. In recent years, robotic chemists have become an important area of study to improve test efficiency, data accuracy, and process reliability. This project addresses the problem of autonomous manipulation of chemistry containers such as test tubes and flasks in a safe and optimal manner. While most existing solutions cannot complete this task due to the complicated environments in laboratories, this project proposes to develop an RM system with optimal control and safety guarantees that can lead to increases in efficiency and reproducibility of laboratory experiments. A visual servoing via RLMPC framework ensuring fast, smooth, robust, and safe operation of the RM is intended to be developed. The overall RLMPC framework consists of two parts: The RL module for achieving optimal control performance, and the MPC module ensuring safe and robust operation.

Project objectives

Briefly describe the high-level project objectives and outcomes (~150 words).
• Develop a novel and efficient grasping system using a robot manipulator by integrating RL, MPC, and visual servoing in a unified framework. • Apply the developed RLMPC framework to real-world chemistry laboratory tasks such as pouring reagents and transmitting common chemistry containers. • Explore the capability of the RL methods to enhance the robustness of the RM system against the model mismatch, external disturbances, or other unexpected issues. • Perform theoretical analysis, simulation verifications and experimental tests of the proposed methods for identification and quantification of the closed-loop performance of the developed system. • Investigate solutions to improving the computational efficiency of solving the online RLMPC optimization problem to resolve the implementation limitation of the proposed method. • Create a generic solution and platform by combining both the advantages of learning and optimization that can also be used for a wide range of applications such as bio-reactors, intelligent materials processing control, etc. • Assess the robustness and efficiency of RLMPC versus standard RL.

Alignment with AI for Design

What is being designed (~100 words)?
An RLMPC framework unifying RL and MPC for the RM system to conduct the grasping task is to be designed. In this combined RLMPC framework, MPC is responsible for ensuring the reliable and safe operation of the RM by restraining the movement of joints, and RL provides a solution to the control of complex manipulators that are difficult to model by both assisting in offline training and serving as a tuning tool for online adjusting MPC design parameters to achieve optimal grasping performance. Therefore, the RLMPC framework can help facilitate safe and efficient control system design of robots carrying out tasks in general-purpose chemistry labs.
How is AI integral to the design (~100 words)?
As MPC is known as a model-based control strategy, the control performance of MPC may be degraded when the model used in MPC is not accurate enough mainly due to external disturbances, model mismatch, changing environments, etc. RL is then motivated to be incorporated into the MPC framework to adjust the parameters of the MPC controller for performance enhancement in the presence of model mismatch. For robot manipulators especially for those with hard system constraints induced by operation environments, RL will maintain the recursive feasibility of the MPC optimization problem while updating associated design parameters online to improve the control performance.
How can the developed methods be applied to other problems (~100 words)?
The proposed RLMPC framework studied in this project is originally developed for RMs with high precision. However, the design strategies used for this project are widely applicable to general autonomous systems, such as unmanned aerial vehicles since the proposed method only requires the robot model with a certain level of accuracy. The model mismatch and unknown working environment can be learned from the data generated and collected during the online control process by using the RL mechanism in the RLMPC framework. Different control objectives and practical constraints in other problems can be considered by appropriately formulating the

MPC optimization problem.

Project linkage to master project

Explain how the project fits within the master project to which it is associated (~100 words).

The unified RLMPC framework proposed in this project for executing complicated however repeated tasks autonomously, safely, and optimally via the RM in a material design chemistry laboratory will be developed by integrating AI into the model-based optimal control scheme. This AI-assisted control framework can be further extended to conduct similarly complicated and repeated tasks using suitable robots in biological applications such as developing biological sensors, materials, and catalysts. The overall AI-integrated system design will significantly improve performance, efficiency, flexibility, and reliability for a wide range of domains such as intelligent material processing control, medical applications, life science research, biotechnology, and bioengineering.