NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

MS4671 – High Throughput Experimental Methods for Materials Discovery

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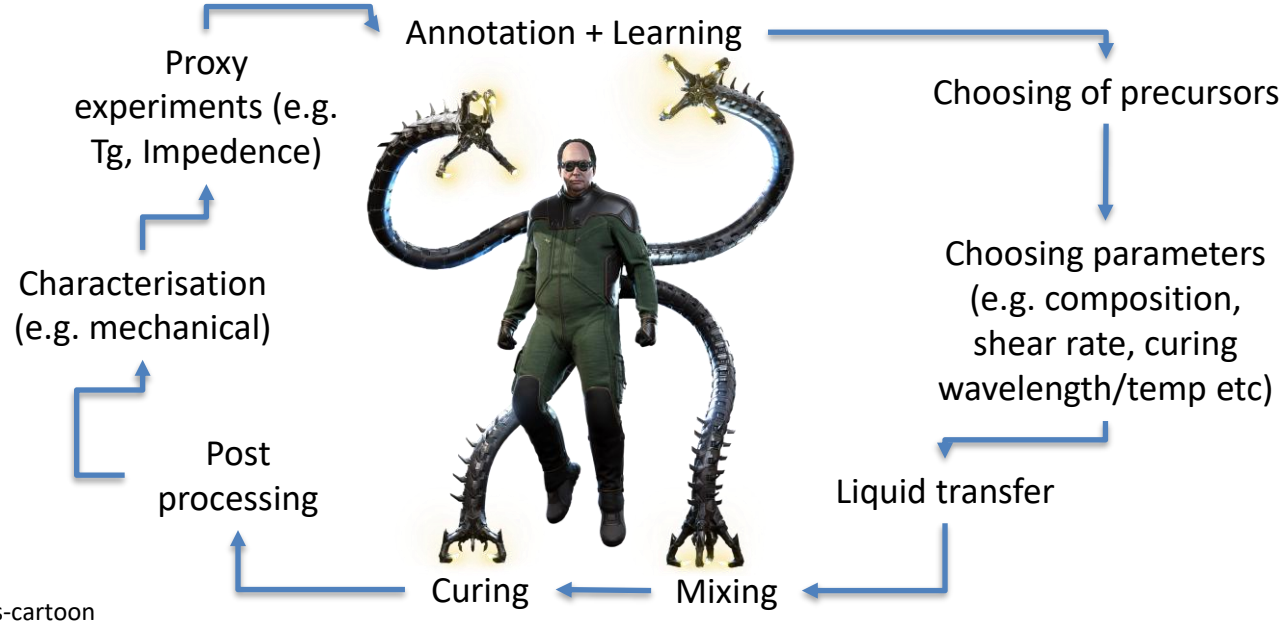
Today's class

- Part 1: Introduction to High-Throughput Experimentation (20 mins)
  - Introduction to High Throughput experimentation (10 mins)
  - Opentrons automated pipetting robots (5 mins)
  - OpenCV framework (5 mins)

- Part 2: Automated mixing of food die using Opentrons
  - Opentrons automated solution mixing (1hr)
  - Producing rainbow colors via automated mixing code (In-class quiz) (1hr)
  - OpenCV image recognition (30mins)
  - Homework (Making a target color via BO and automated solution mixing) (30mins)

High Throughput Experimentation

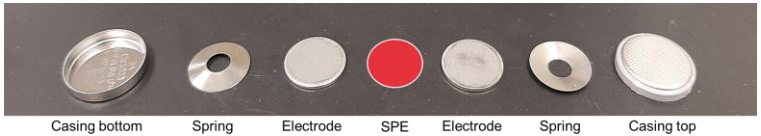
What is high throughput experimentation and why is it important?



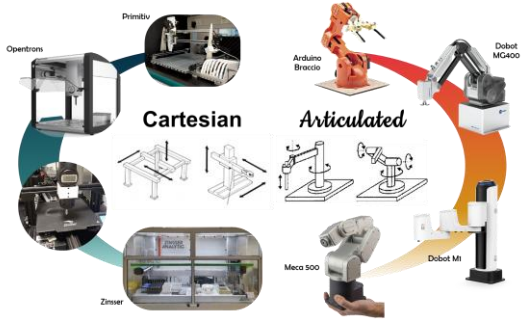
https://www.vecteezy.com/free-vector/octopus-cartoon

Types of modules used in HTE

Machines for making things out of stuff

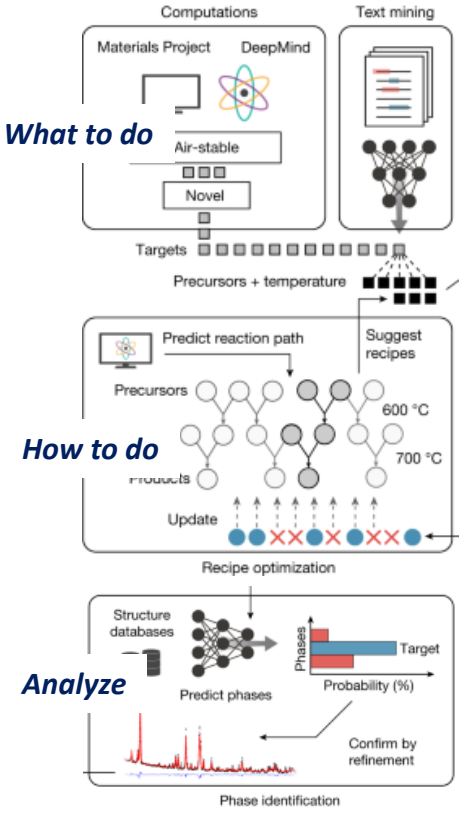


Machines for moving stuff



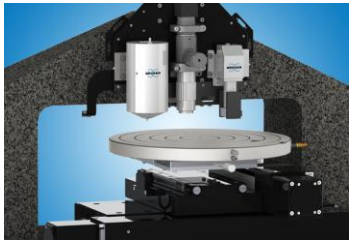
Machine for Testing

Decision-making brain



Types of experimental techniques in HTE

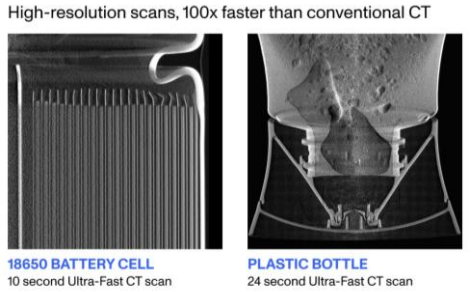
- Point-wise experiments (e.g. mechanical, spectrum analysis, electrical etc…)
- Parallel/Simultaneous experiments (e.g. impedance spectroscopy, gas adsorption etc…)
- Proxy experiments (Optical, electrical measurements)
- Ultrafast analysis



Nanoindenter

Potentiostat

Hyperspectrum

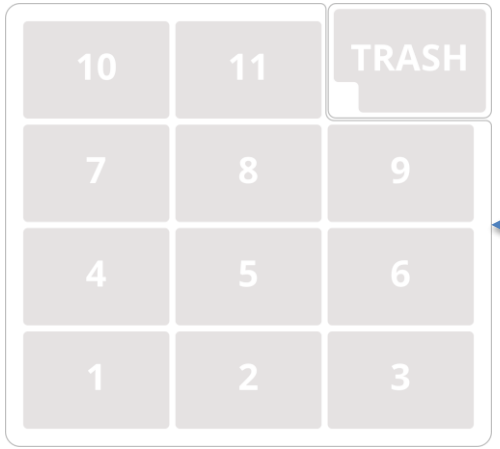


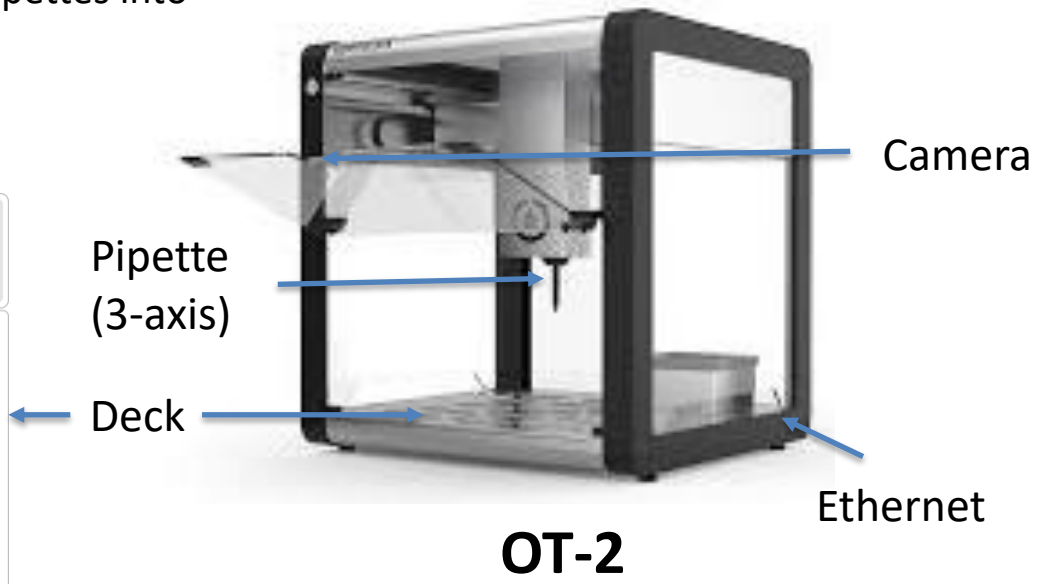
Ultrafast CT

https://www.bruker.com/en/products-and-solutions/test-and-measurement/nanomechanical-test-systems/hysitron-ti-980-nanoindenter.html
https://www.biologic.net/product_category/potentiostats-galvanostats/
https://www.lumafield.com/product-feature/ultra-fast-ct-scanning
Wikipedia

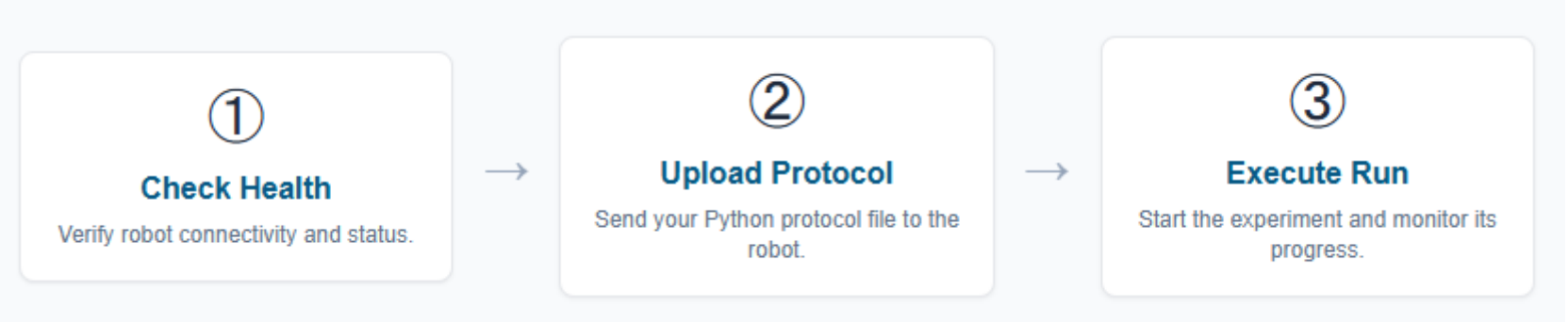
Introduction to Opentrons

- 3-axis Liquid handling robot
- Picks liquid from reservoir (resource), pipettes into receptacle, disposes tips in trash
- Python controlled
- Standardized labware

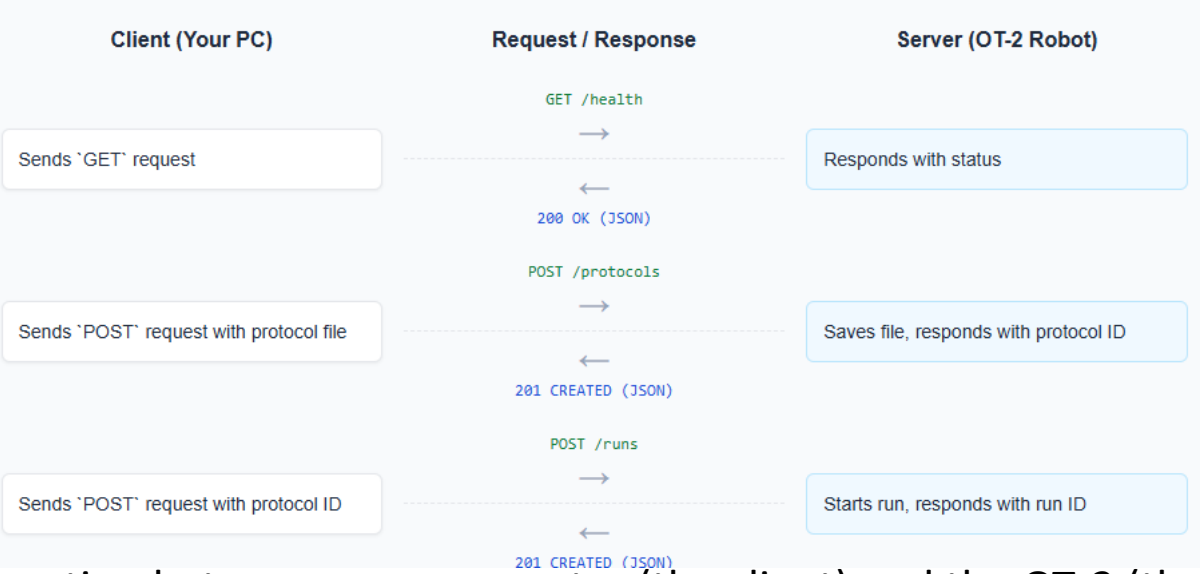




Core Workflow Overview of OT2

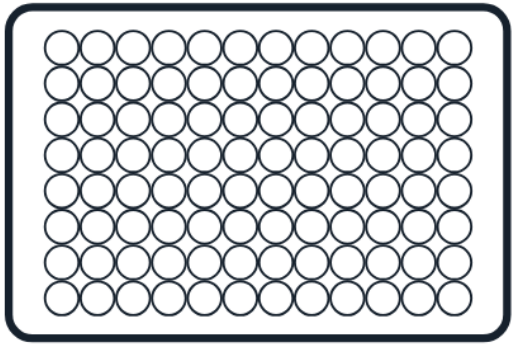


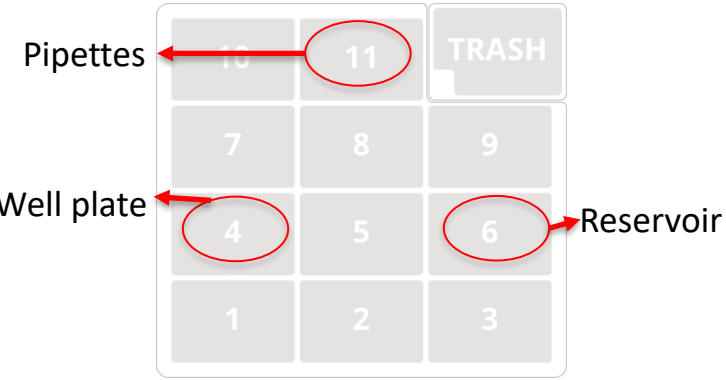
Communication protocol using Rest API

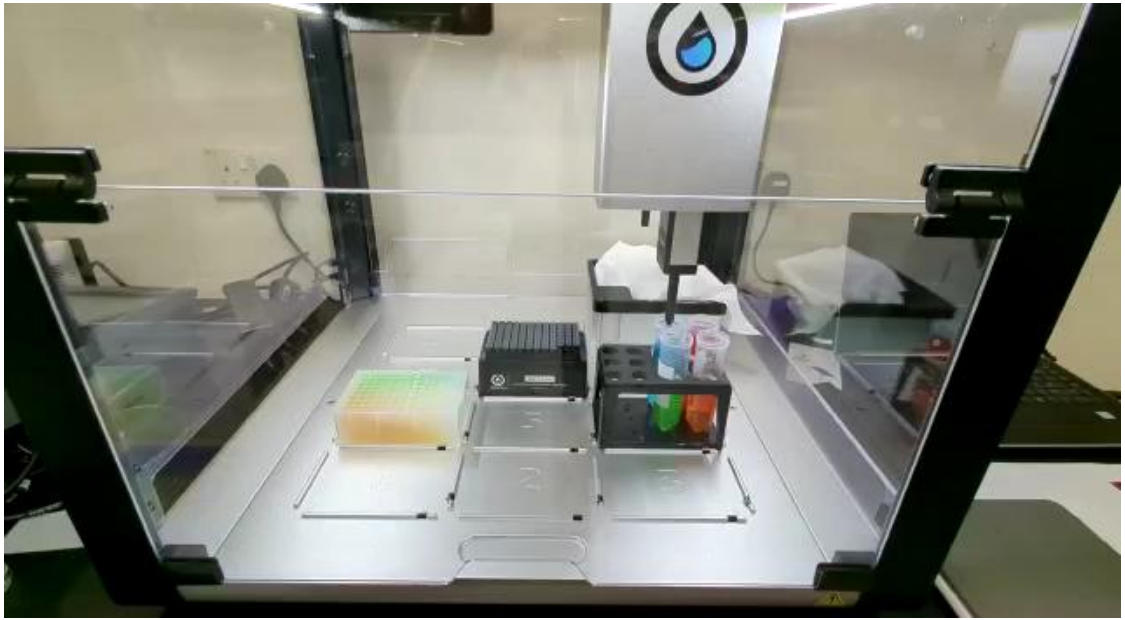


- The interaction between your computer (the client) and the OT-2 (the server) is managed through a REST API.
- Scripts sends HTTP requests to specific URLs on the robot, and the robot responds with JSON-formatted data.

Automated colour mixing using Opentrons







- Amount of colour x transferred to each well
- Efficiency in liquid transferring

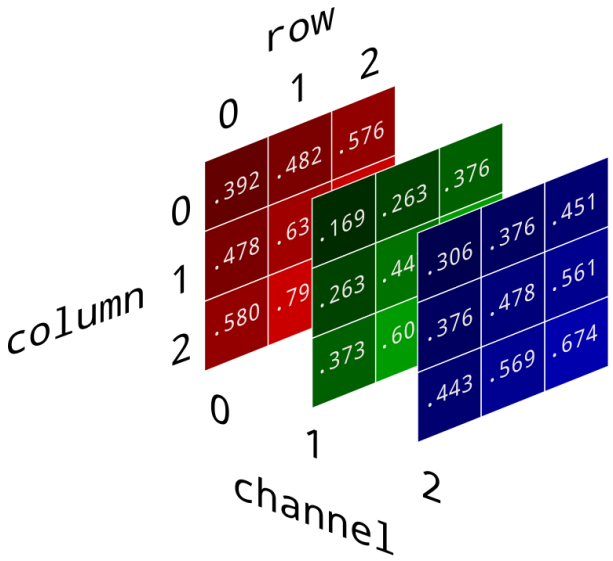
OpenCV Library

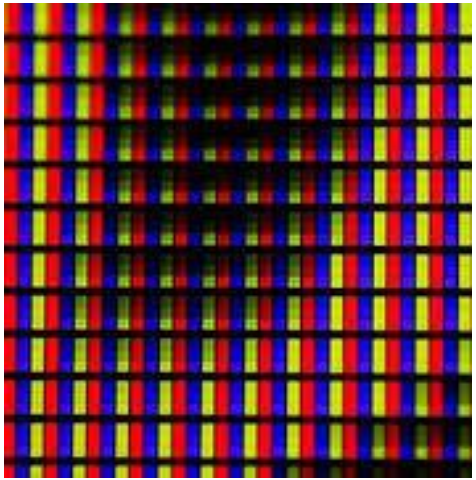
- Image manipulation
  - Read and display
  - Color space and channel manipulation
  - Resize, rescale, cropping
  - Transformations
  - Draw and Masking
- Object and Face detection
  - Contour, thresholding, and edge detection
  - Basic item detection and recognition
- Connecting with AI modules

Open Computer Vision Library

pip install opencv-python
Python >=3.6

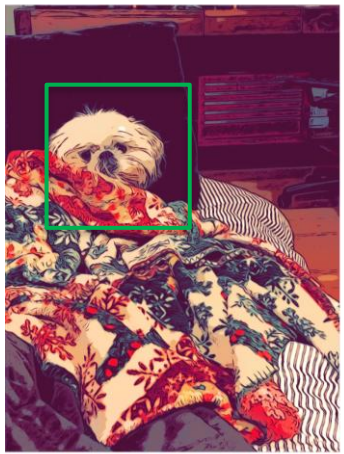
Image





https://brandonrohrer.com/convert_rgb_to_grayscale.html

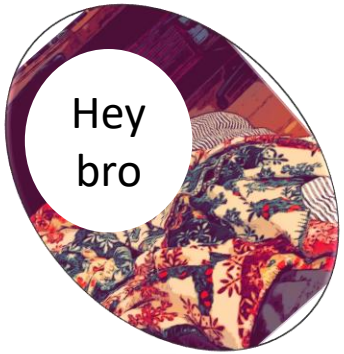
Functionalities



Img

Resize

Crop



Mask & rotate

Transform

CVT

Contour / Edge

https://brandonrohrer.com/convert_rgb_to_grayscale.html

In-class Quiz (60mins)

(Follow the code provided to achieve automated color mixing)

1. Modify the code provided (protocol_modified.py) to achieve automated “rainbow” color mixing in a row.
2. Example code can be found in https://github.com/dannyzekunren/MS4671

Homework

Using active learning to make a target color

Wee4_homework.ipynb can be found in

https://github.com/dannyzekunren/MS4671

1. Target color: RGB values. (55,150,40), or you can random generate
2. Active Learning: Design an efficient algorithm to control the Opentrons to mix automatically and approach this color.
3. Operation: Demonstrate the code on Opentrons.

Automated Loops

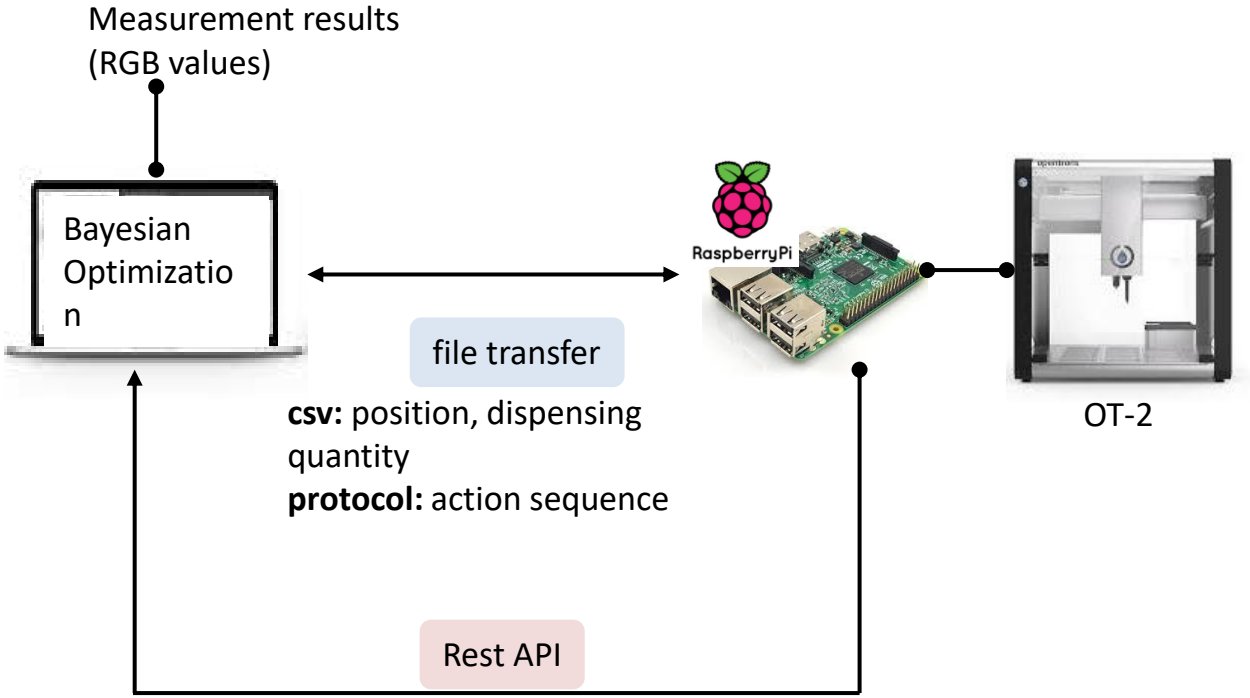
Generate Instructions

Run Protocols

Remote commands to OT2

Measurements and Analysis

Full Feedback Loop

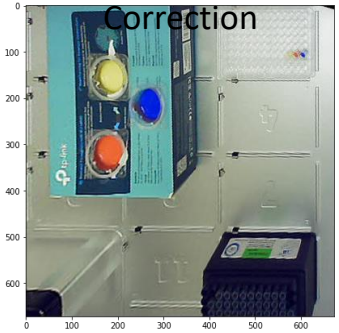


Send a message when completing the actions: `aiohttp`

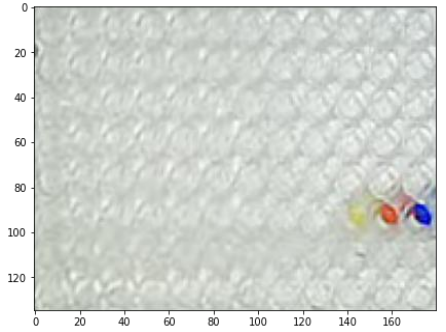
Color mixing

Raw Image

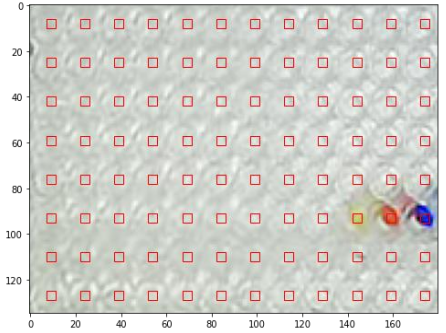
Perspective Correction



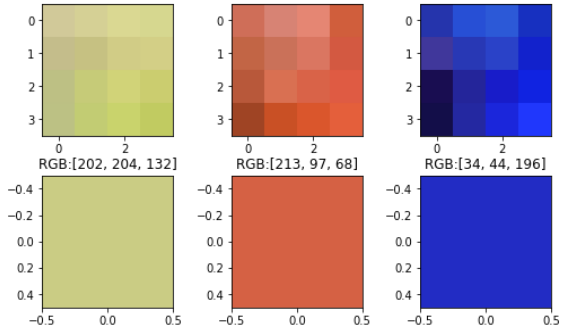
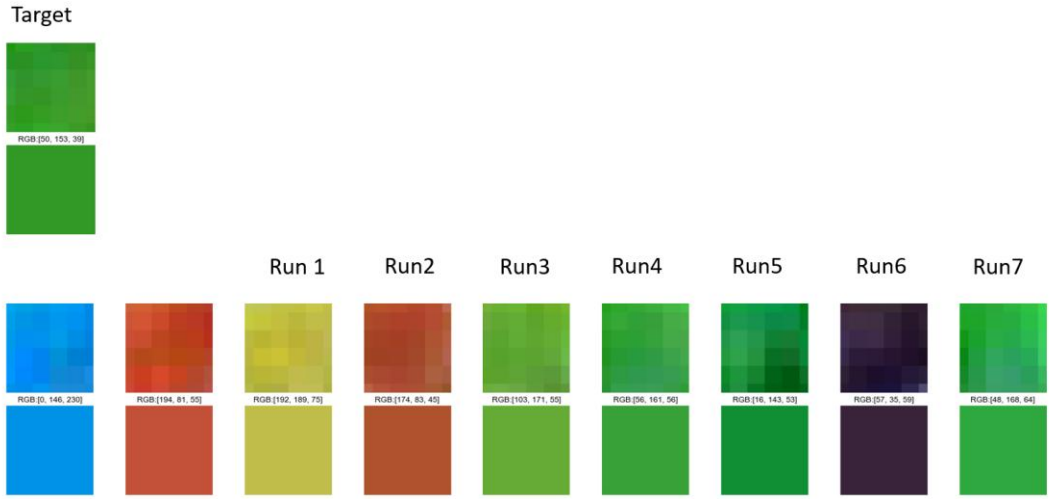
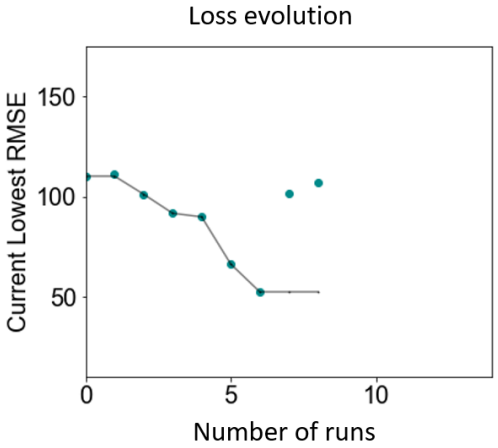
ROI Cropping



Sample Isolation



RGB Extraction



The expected results