HANLTEN

Python in Lab Automation

Building on solid ground

OST Rapperswil, 17 October 2024

J.Rast (@jrast on ())

Outline

- 1 How Hamilton got started with Python
- 2 ... and where we are today
- 3 A glimpse into the future





How Hamilton got started with Python



Providing Solutions since 1950

HAMILT®N





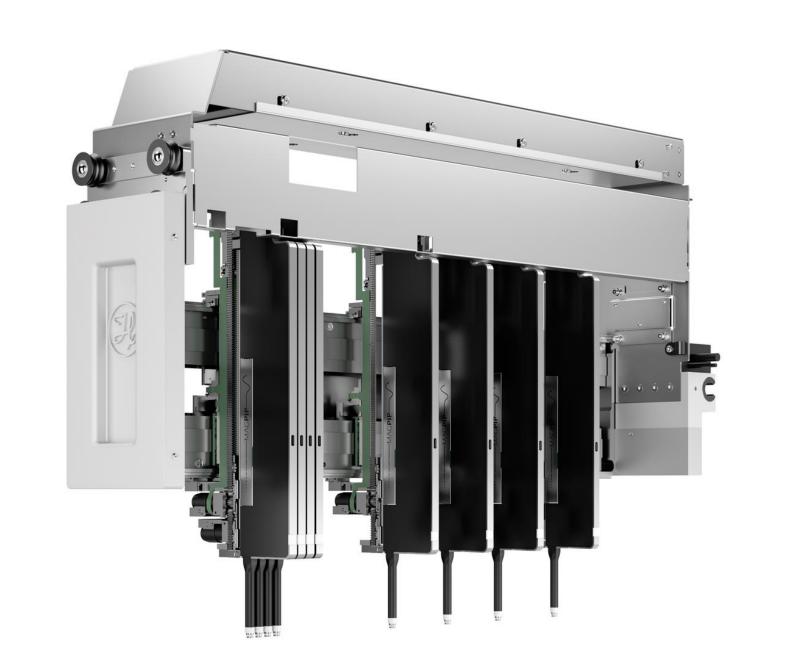


Innovative pioneer in the fields of automated liquid handling, sample management, process sensors, laboratory equipment and ventilators.

Hospitals, laboratories, Biobanks and other institutions across the globe rely on us, our products and services.



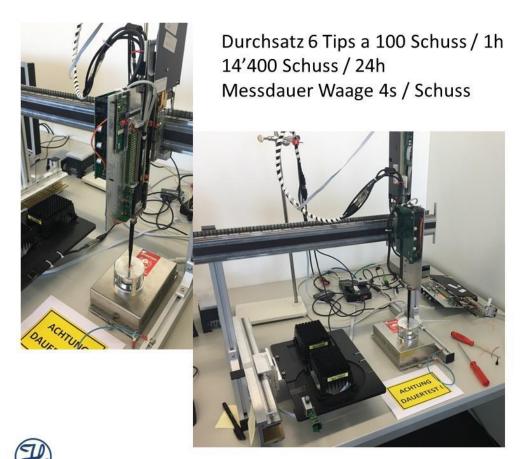






Want to find out more? Visit https://www.youtube.com/watch?v=DIPl3p4rb8w





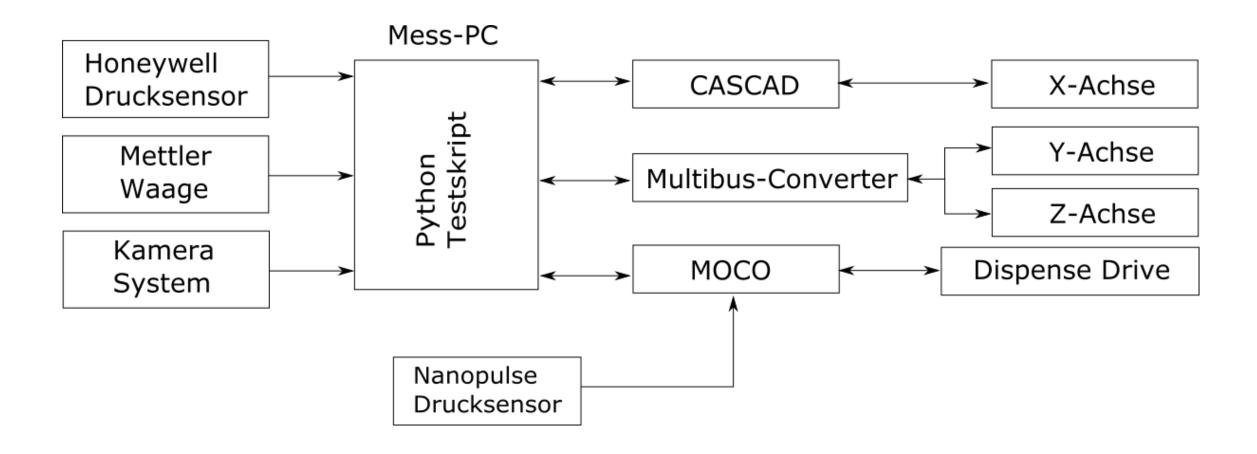


Automatischer Report nach 100 Aliquotes/Tip per Mail

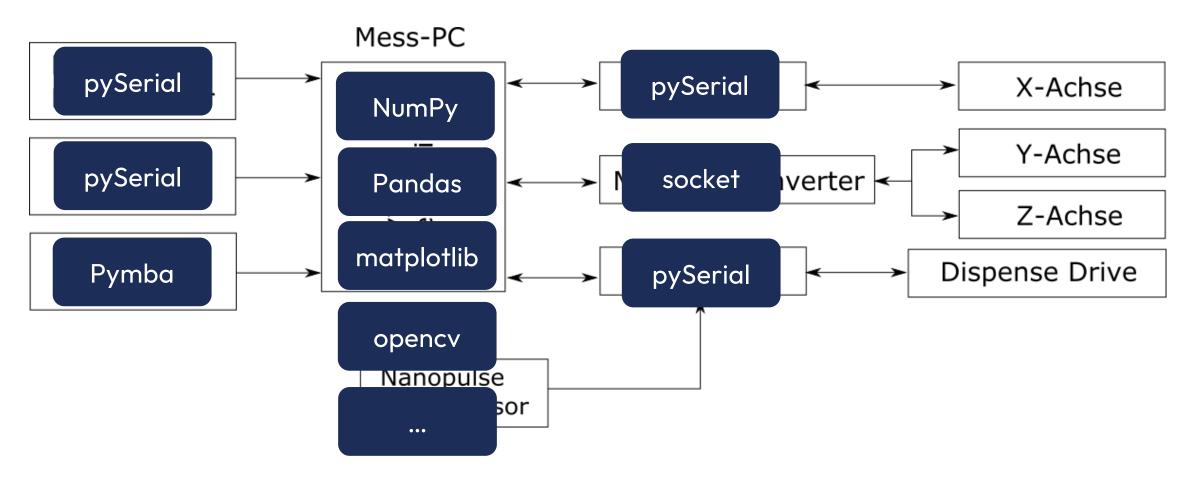
Datenerfassung aller relevanten Parameter und Messgrössen in Datenbank Engineer

Because badass miracle worker isn't a job title









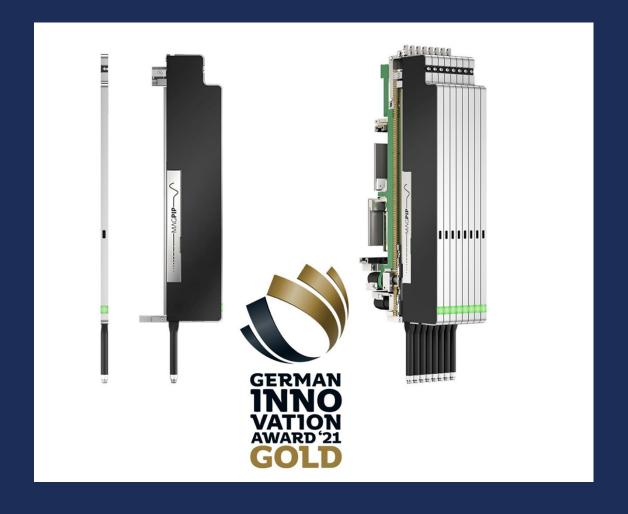


```
print("Writing Moco Config")
moco.read(cmds.SERR) # Dummy Read System Error
for cmd in cmds.writable():
    if hasattr(cmd.write, 'default') and cmd.write.default is not None:
        response = moco.write(cmd.number, cmd.write.default)
        if response.error:
            print("Failed Writing {} = {} to Moco".format(cmd.name, cmd.write.default))
print("Moco Alignement")
moco.action(cmds.STEP, -50000)
moco.wait ready()
moco.action(cmds.ALGN, 0)
moco.wait ready()
if moco.read(cmds.DERR).data > 21:
    print("Moco Alignement Failed")
print("Moco Init")
moco.action(cmds.IPOS, 200000)
moco.wait ready()
if moco.read(cmds.DERR).data > 0:
    print("Moco Init failed")
print("Move to first Position")
moco.action(cmds.TPOS, -1000)
moco.wait ready()
if moco.read(cmds.DERR).data > 0:
    print("Moco Move failed")
```



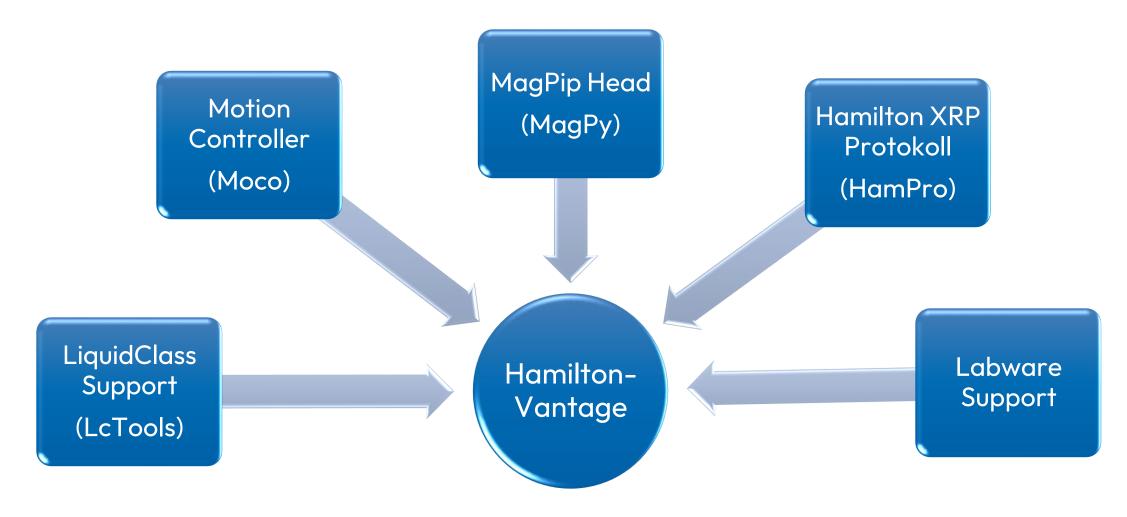
Retrospective

- It was a mess:
 Code was changed fast and written mostly
 as «spaghetti code»
- It was a bit like open-heart surgery:
 If something broke, the whole system came to a halt.
- But we were fast!











- Parallel Sampling of ~60 internal signals in FW with up to 20kHz Sampling Rate
- Transfer via USB using python-libusb1 in real-time
- Context-Manager to start / stop the acquisition even when something goes wrong.
- Data Acquisition directly into a Pandas DataFrame
- Optional live data processing with up to 1kHz



```
with ana.start(fs=0.5) as df:
    arm.aspirate clld lw list lc(
        asp source,
       target volume,
       clld sens=2,
       liquid cls=liquid cls,
       z cmd start=Z USB,
       z cmd end=Z USB,
       # Set Liquid Tracking enabled
       ct=[CONTAINER ID] * 8,
        ze=[1] * 8,
   response = arm.send cmd("WMVL")
   liquid_level = arm.units.Z.arm2mm(response.vl[channel_idx])
    print(f"Liquid Level: {liquid level:.1f}mm")
    data["liquid levels"].append(liquid level)
   weight after asp = helpers.get weight()
   data["weights after asp"].append(weight after asp)
```



- Working with abstract / logical positions
- Geometry modeled with NumPy
- Visualisation with vtk (work in progress ...)

```
with ana.start(fs=0.5) as df:
    arm.aspirate clld lw list lc(
        asp source,
       target volume,
       clld_sens=2,
       liquid cls=liquid cls,
       z cmd start=Z USB,
       z cmd end=Z USB,
       # Set Liquid Tracking enabled
       ct=[CONTAINER ID] * 8,
       ze=[1] * 8,
   response = arm.send_cmd("WMVL")
   liquid_level = arm.units.Z.arm2mm(response.vl[channel_idx])
   print(f"Liquid Level: {liquid level:.1f}mm")
   data["liquid levels"].append(liquid level)
   weight after asp = helpers.get weight()
   data["weights after asp"].append(weight after asp)
```

- Complex behavior abstracted away into "Liquid Classes"
- Access to "Liquid Database" of the user software through pyodbc

Access to low level functionality still retained

```
with ana.start(fs=0.5) as df:
    arm.aspirate clld lw list lc(
        asp source,
       target volume,
       clld_sens=2,
       liquid cls=liquid cls,
        z cmd start=Z USB,
       z cmd end=Z USB,
       # Set Liquid Tracking enabled
       ct=[CONTAINER_ID] * 8,
       ze=[1] * 8,
    response = arm.send cmd("WMVL"
   liquid_level = arm.units.Z.arm2mm(response.vl[channel_idx])
    print(f"Liquid Level: {liquid level:.1f}mm")
    data["liquid levels"].append(liquid level)
   weight after asp = helpers.get weight()
   data["weights after asp"].append(weight after asp)
```

- Clean libraries for our devices
- Complexity is abstracted away
- Even non-programmers can at least understand, or reason about, what a script is doing
- With CoPilot & Co. they will soon be able to write their own scripts





The Use of AI-Robotic Systems for Scientific Discovery

Article | Open access | Published: 20 December 2023

Autonomous chemical research with large language models

Daniil A. Boiko, Robert MacKnight, Ben Kline & Gabe Gomes

✓

Nature 624, 570–578 (2023) Cite this article

132k Accesses | 109 Citations | 940 Altmetric | Metrics

Article | Published: 08 July 2020

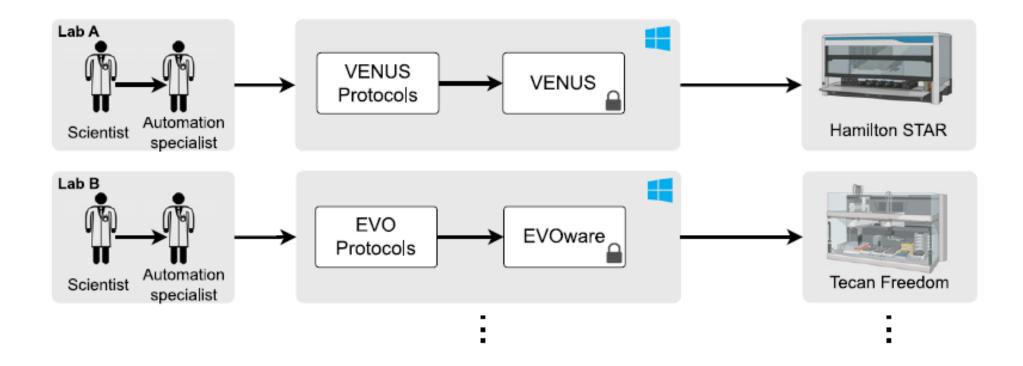
A mobile robotic chemist

Benjamin Burger, Phillip M. Maffettone, Vladimir V. Gusev, Catherine M. Aitchison, Yang Bai, Xiaoyan Wang, Xiaobo Li, Ben M. Alston, Buyi Li, Rob Clowes, Nicola Rankin, Brandon Harris, Reiner Sebastian Sprick & Andrew I. Cooper

Nature 583, 237–241 (2020) | Cite this article

89k Accesses | 717 Citations | 1145 Altmetric | Metrics







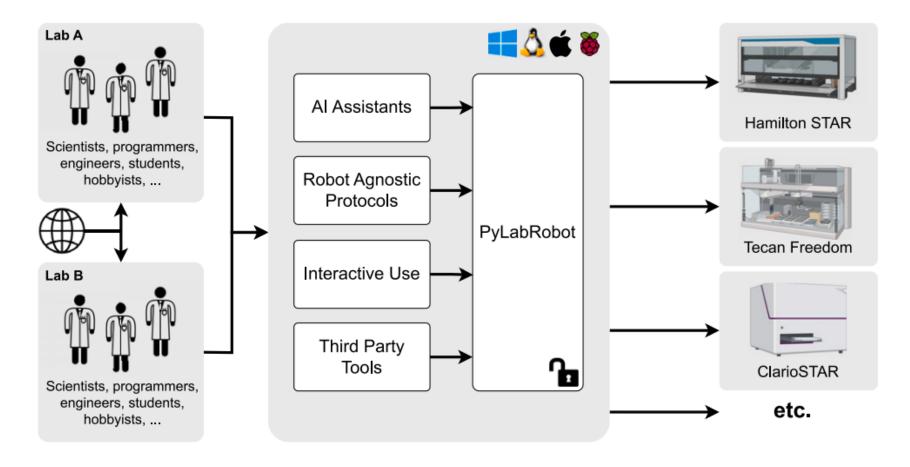
PyLabRobot: An open-source, hardware-agnostic interface for liquid-handling robots and accessories

```
Rick P. Wierenga 1,2 · Stefan M. Golas 2 · Wilson Ho 2,3 · Connor W. Coley 4 · Kevin M. Esvelt 2,5 ⊠
```

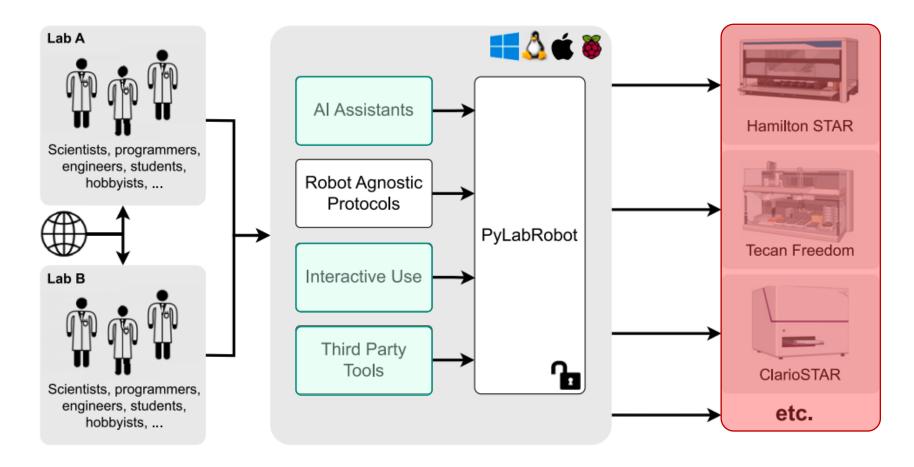
Affiliations & Notes ✓ Article Info ✓



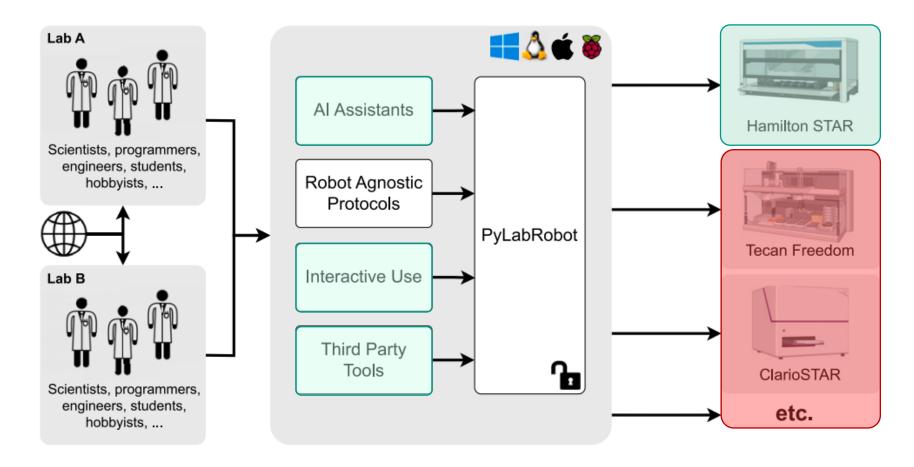


















Do you have any questions?

Hamilton Americas & Pacific Rim

4970 Energy Way Reno, Nevada 89502 USA Tel: +1-775-858-3000 Hamilton Europe, Asia & Africa

Via Crusch 8 CH-7402 Bonaduz Tel: +41 58 610 10 10