

Experimental Design and Operation Strategies for Accelerated Bioprocess Development



M. Nicolás Cruz B.

motivation

self-driving bio-innovation

accelerating Bioprocess Development

objective:

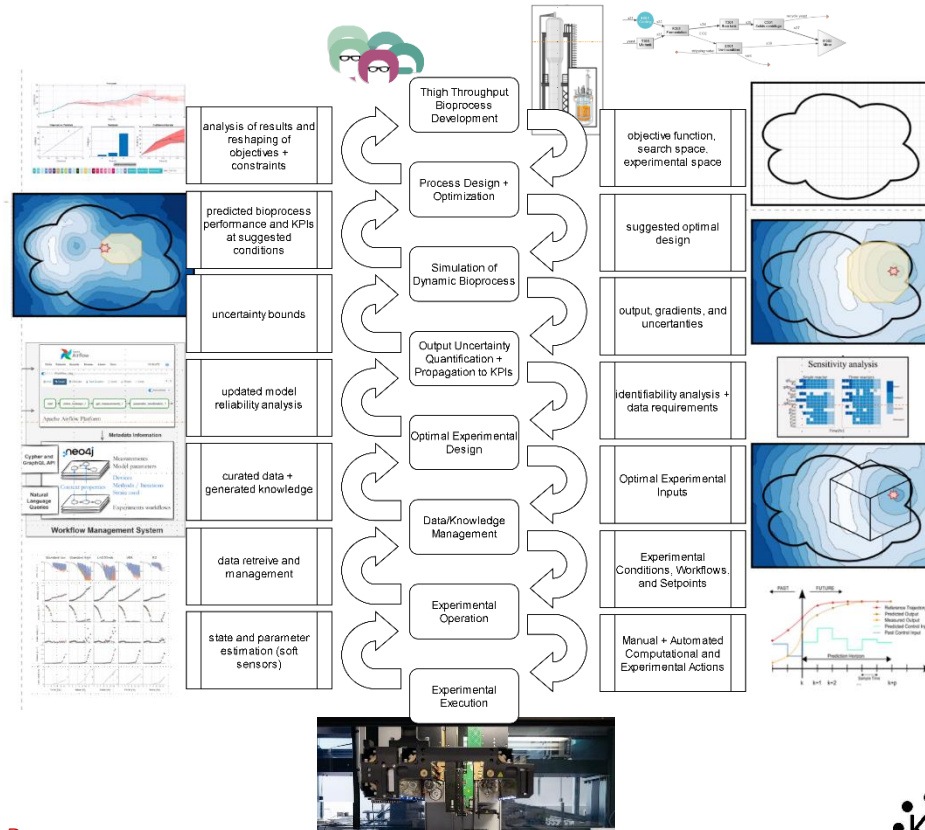
To build the most efficient knowledge generation machinery for the development of new bioprocesses using all necessary existing and emerging technologies

- generate data, information, and knowledge more efficiently
- tightly integrate all existing tools
- take into account the complex dynamics of biomanufacturing
- push collaborative R&D

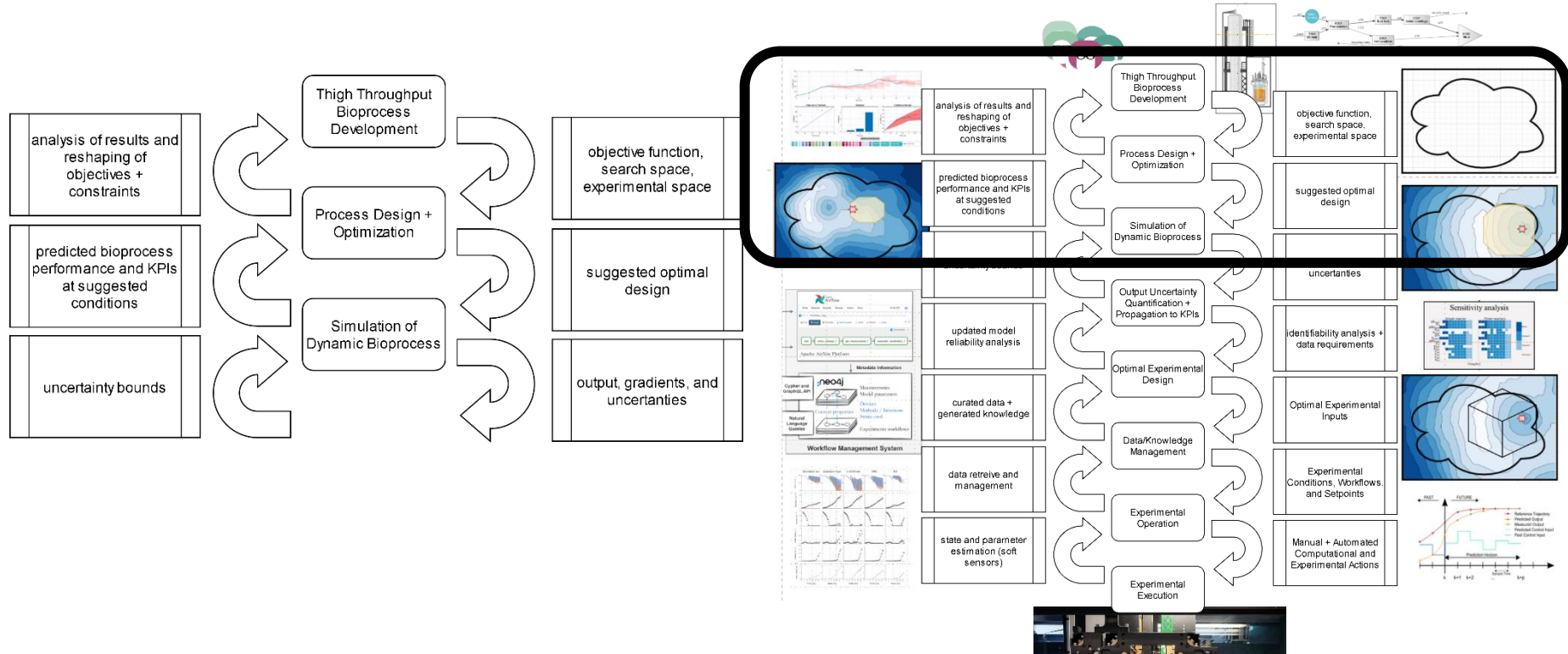


<https://www.nature.com/articles/d41586-022-01618-x>

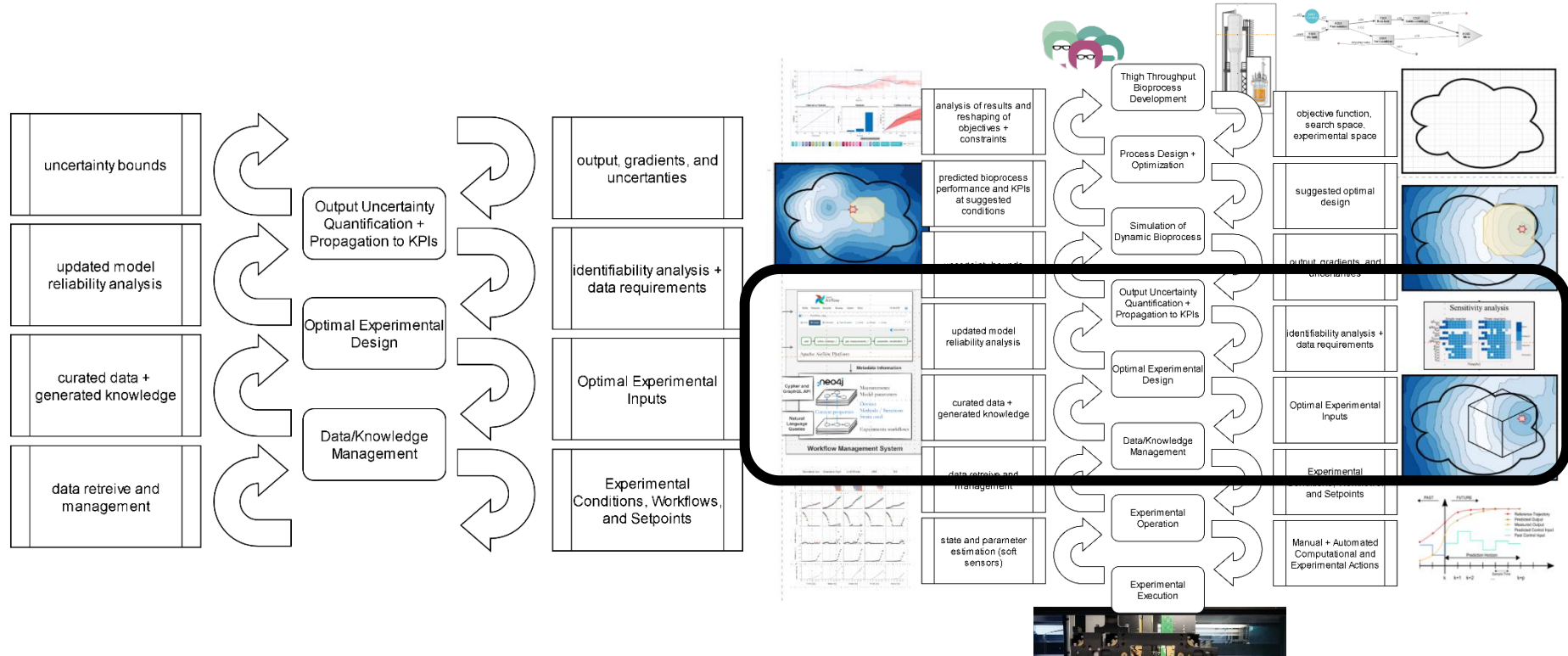
High Throughput Bioprocess Development pipeline

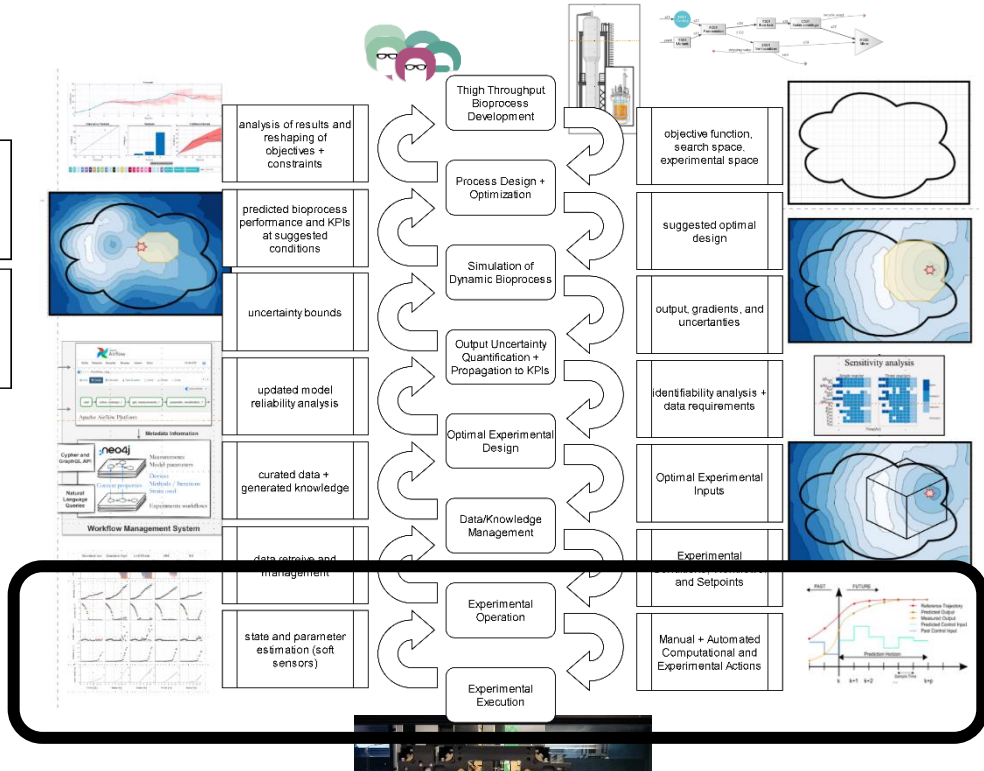


High Throughput Bioprocess Development pipeline

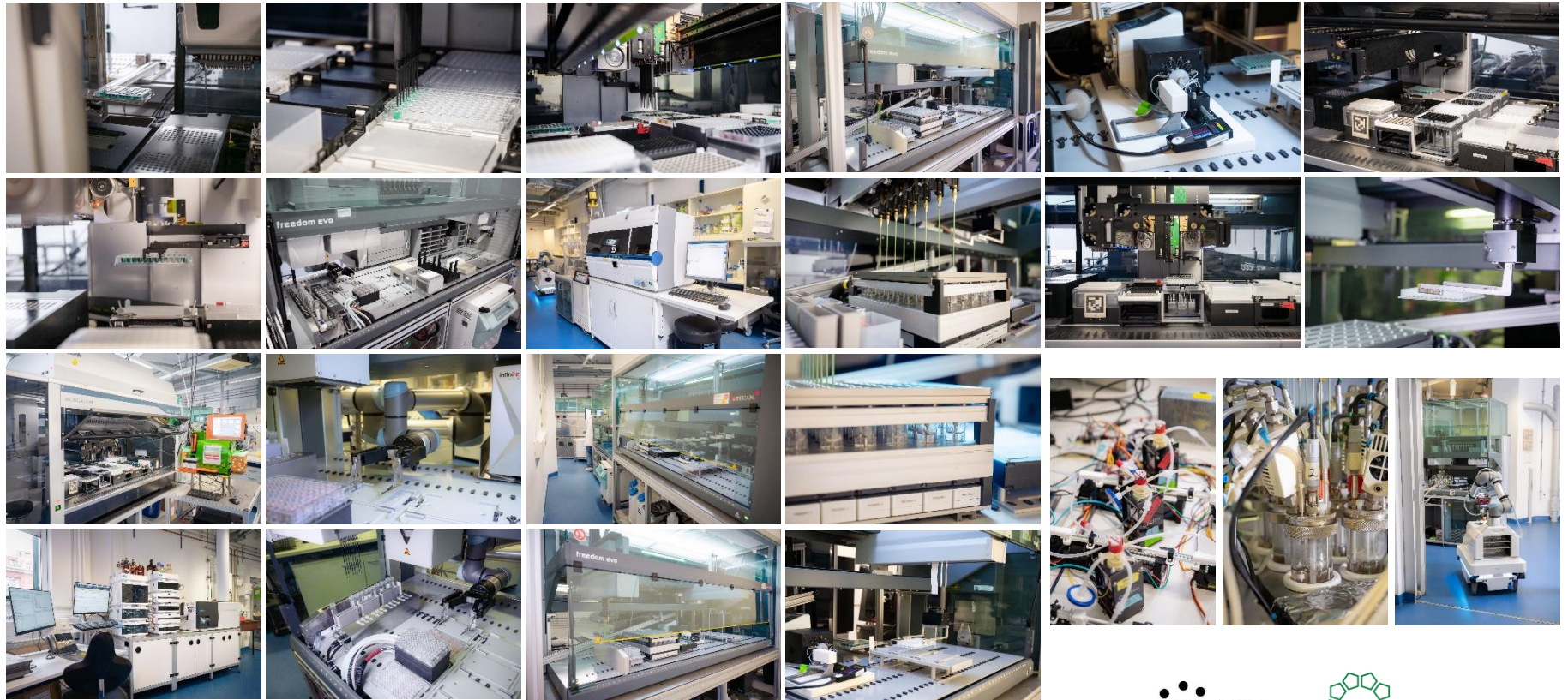


High Throughput Bioprocess Development pipeline





distributed lab environment



making development faster



Annina
Kemmer



Niels Krausch



Simon Seidel



Lucas
Kaspersetz

... and
more



interconnections of different devices

Liquid Handling / Plate Handling



HT facility

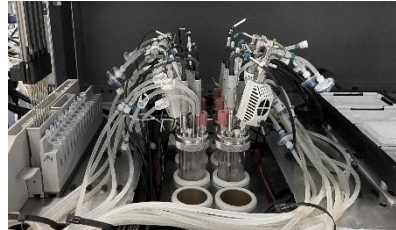


MiLa - mobile lab robot

Cultivation Systems



2mag BioREACTOR 48 - 48 HT
cultivations (10 mL)



h.e.l. BioExplorer 150 - 8 HT
cultivations (100 mL)

Analytics



absorption / fluorescence
(fully automatized)



cell analysis
(semi automatized)



Roche Cedex Bio HT analyzer -
HT analysis of substrates,
metabolites, products
(semi automatized)



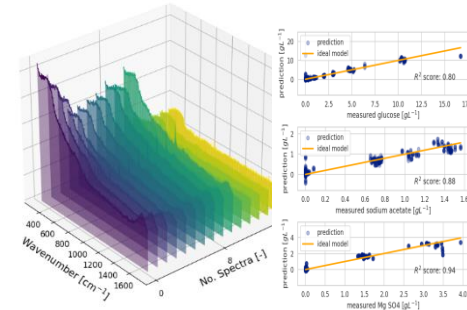
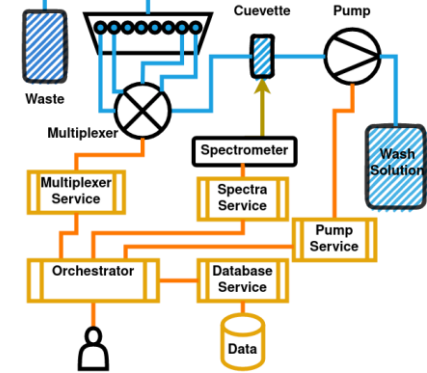
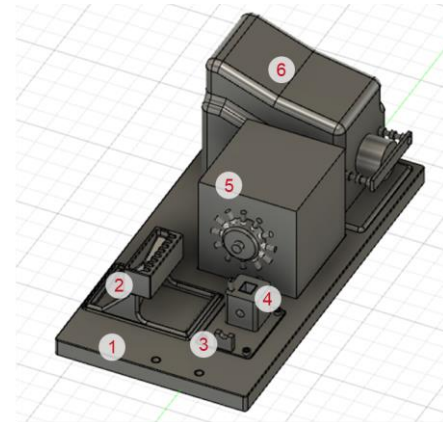
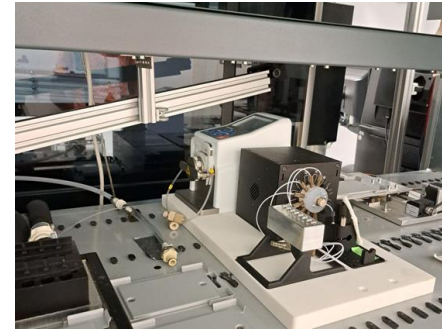
revvity LabChip GXII Touch -
protein characterization
(semi automatized)

...

8 parallel sampling RAMAN in LHS



- ✓ Integration of multi-sample-processing framework in Tecan LHS
- ✓ Reliable measurement procedure
- ✓ Microservice architecture
- ✓ Bioprocess spectra evaluation with Machine Learning models

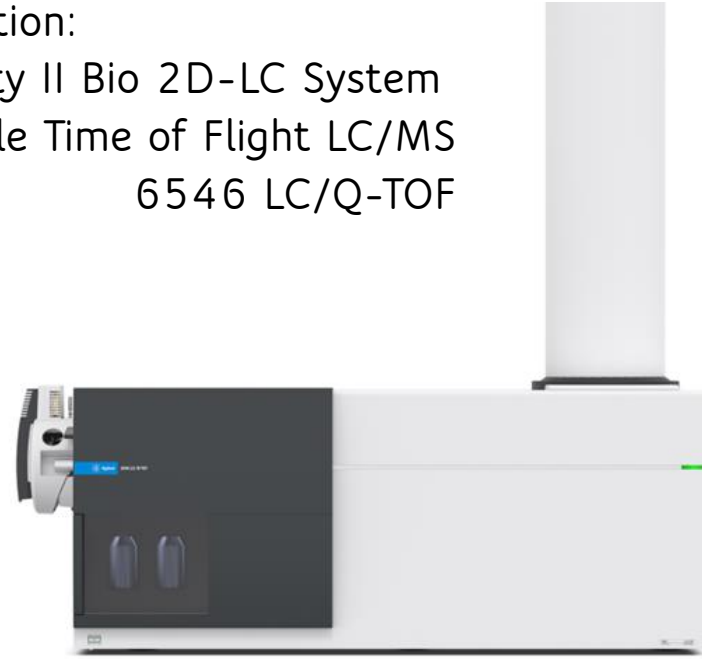


Peter Neubauer: Agilent thought leader Award 2023



under construction:

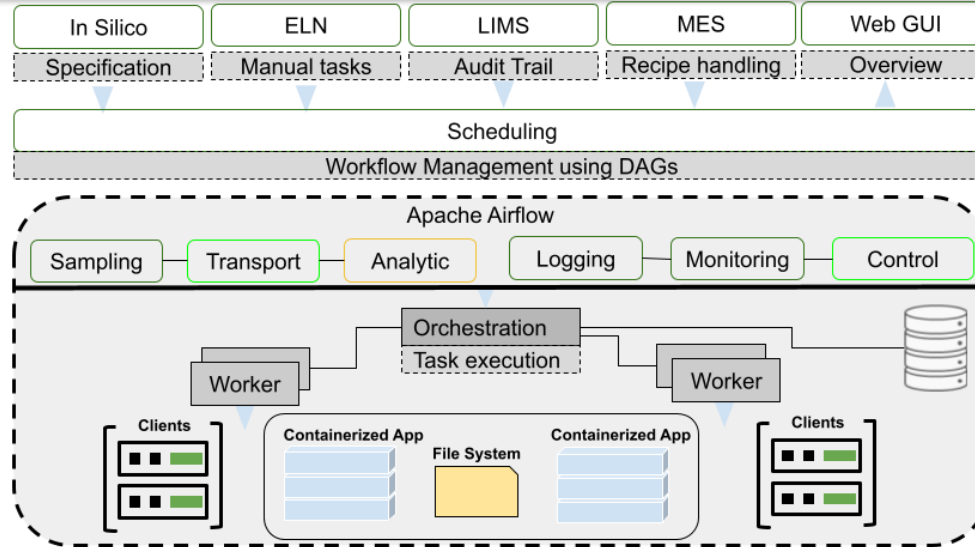
- 1290 Infinity II Bio 2D-LC System
- Quadrupole Time of Flight LC/MS 6546 LC/Q-TOF



User Layer

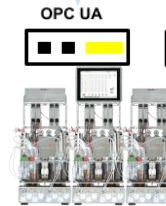


Workflow & Process Control Layer



Standardized Device Interface

Device/ Instrument Layer



making data usable and open

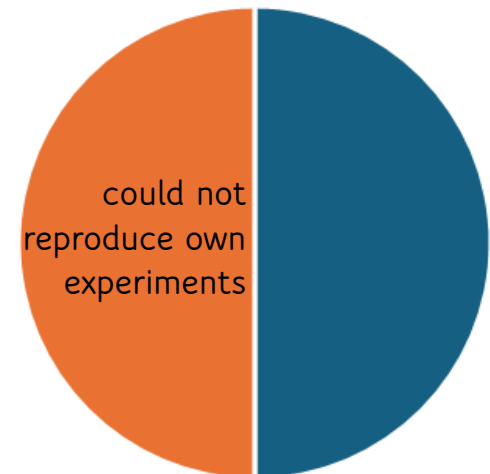
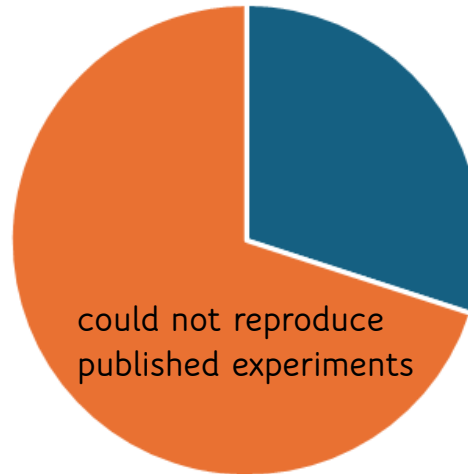
the reproducibility crisis

[Nature: 1,500 scientists lift the lid on reproducibility](#)

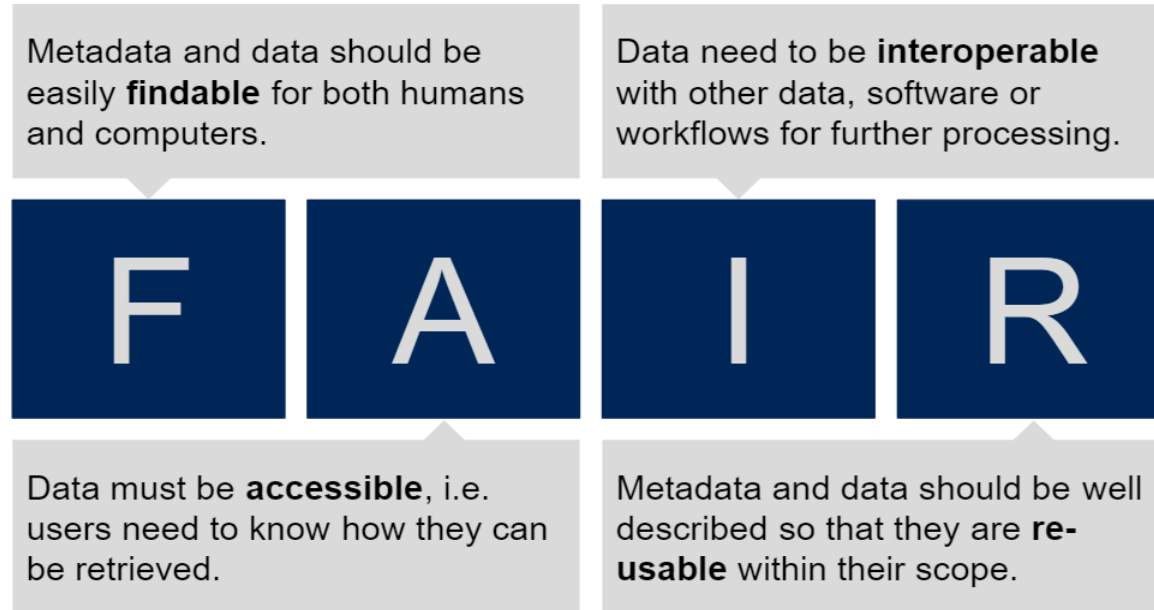
We need:

- *open science and collaborative experimental practices*
- *FAIR experiments*
- *Standards and domain specific ontologies*

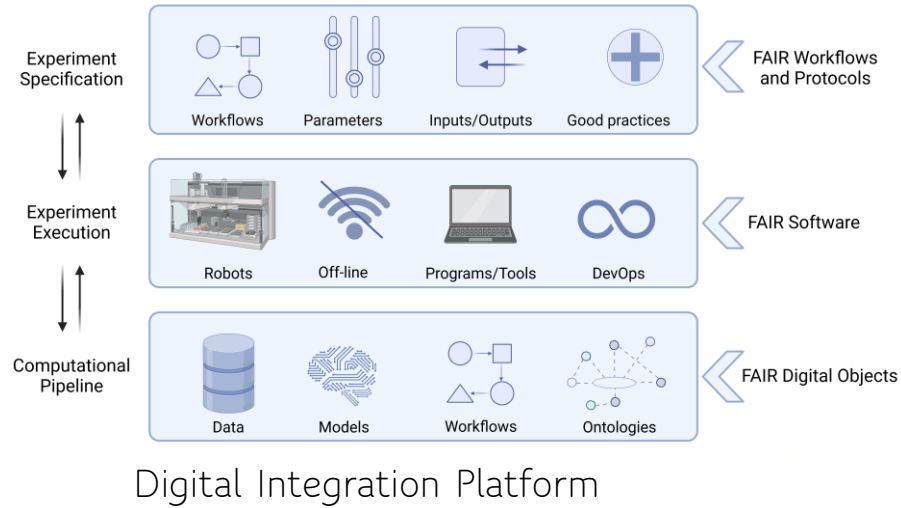
survey with 1,576 researchers



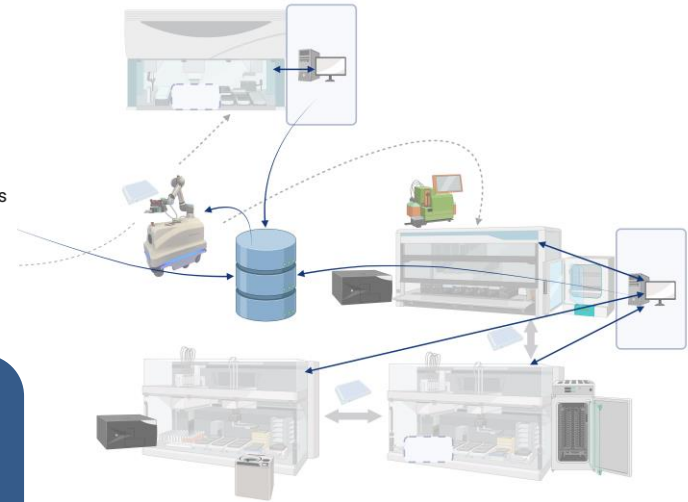
FAIR data principles



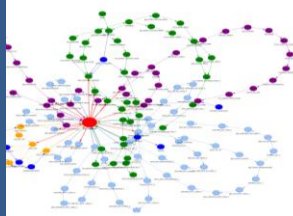
bioprocess R&D – integration of devices and workflows

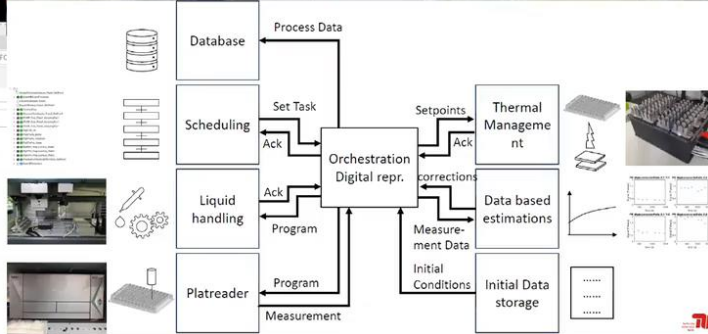


Physical Device Integration



Graph representation







Computers & Chemical Engineering

Volume 187, August 2024, 108720



A workflow management system for reproducible and interoperable high-throughput self-driving experiments

Federico M. Mione ^{a 1}, Lucas Kasperetz ^{b 1}, Martin F. Luna ^a, Judit Aizpuru ^b, Randolph Scholz ^c, Maxim Borisyak ^b, Annina Kemmer ^b, M. Therese Schermeyer ^b, Ernesto C. Martinez ^{a b}, Peter Neubauer ^b, M. Nicolas Cruz Bournazou ^b  



<https://www.sciencedirect.com/science/article/pii/S0098135424001388?via%3Dihub>


Experimental Computational Workflows
☆ Markieren 0

main experimental-computational-workflows
 Verlauf
Datei finden
Code


Update Readme.md
 Mariano Nicolas Cruz Bournazou erstellt vor 4 Monaten
 1a642774

Name	Letzter Commit	Letzte Aktualisierung
📁 dags	Initial commit from experiment	vor 6 Monaten
📁 docs	Initial commit from experiment	vor 6 Monaten
📁 images	Initial commit from experiment	vor 6 Monaten
📁 results	Update plots_summary.md	vor 4 Monaten
📁 .env	Initial commit from experiment	vor 6 Monaten
📁 .gitignore	Initial commit from experiment	vor 6 Monaten
📁 .gitlab-ci.yml	Initial commit from experiment	vor 6 Monaten
📄 Readme.md	Update Readme.md	vor 4 Monaten
📁 docker-compose.yml	Initial commit from experiment	vor 6 Monaten
📁 gitlab-ci.yml	Initial commit from experiment	vor 6 Monaten


Readme.md

A workflow management system for reproducible and interoperable high throughput self-driving experiments

This is the code repository of the work presented in the journal Computers and Chemical Engineering.

Authors

Projektinformation

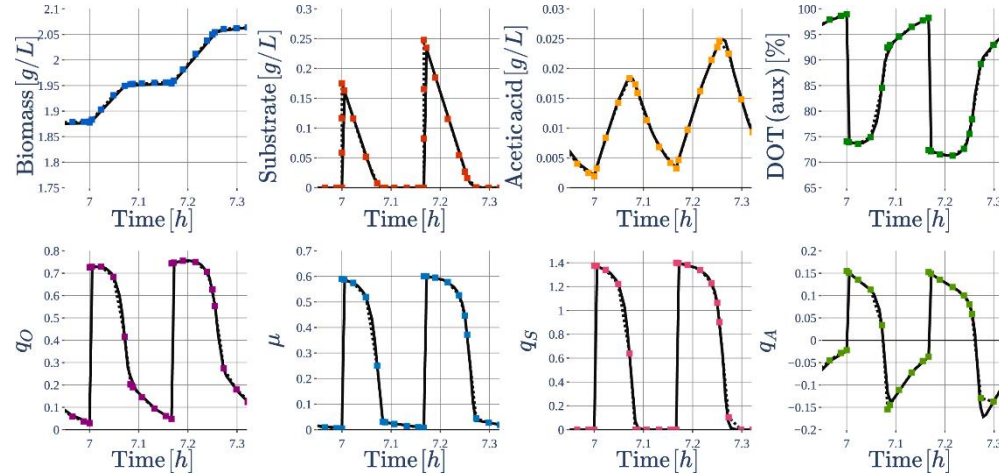
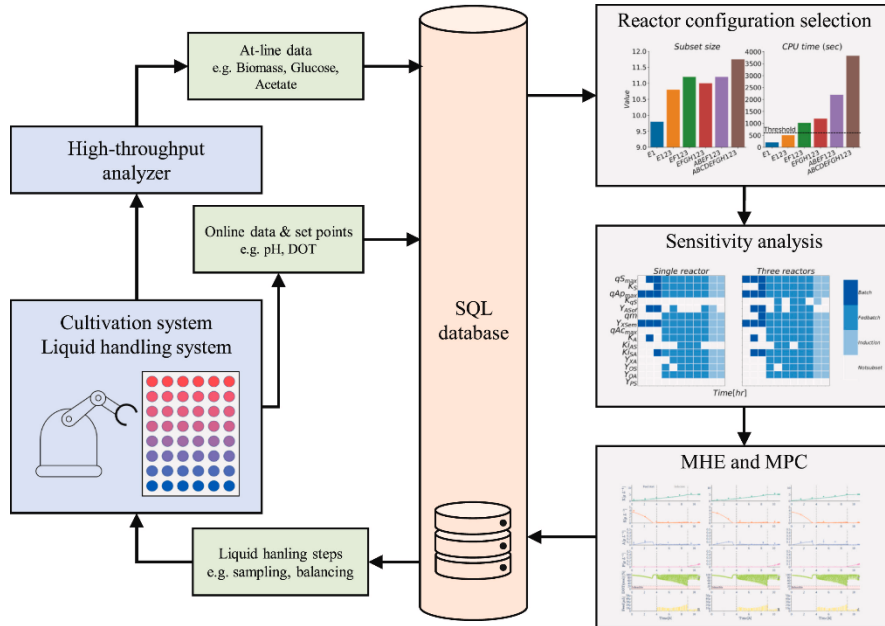
15 Commits
 1 Branch
 0 Tags

README
 GitLab Pages

Erstellt am
 January 24, 2024

integration and deployment in real robotic experiments

nMPC for optimal experimental design



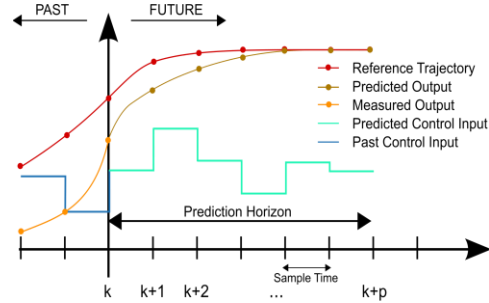
Jong Woo Kim



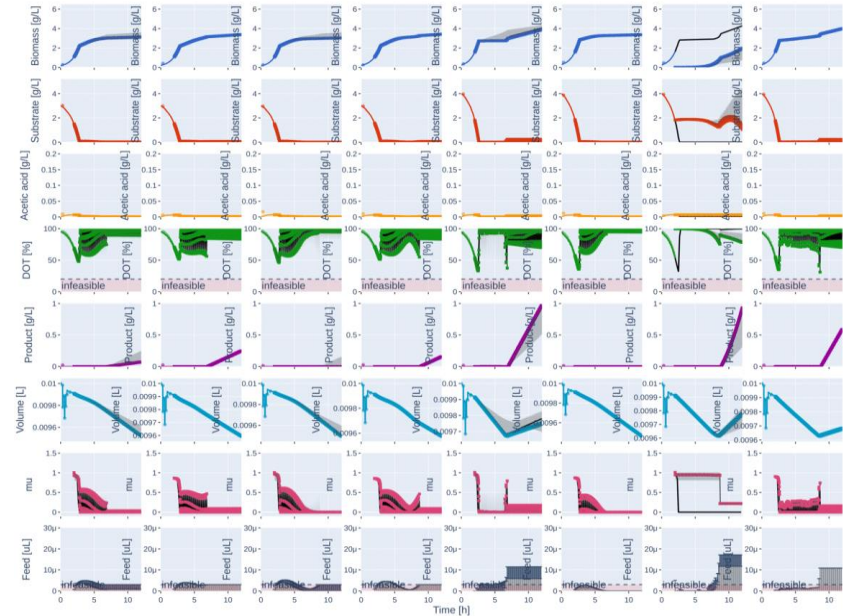
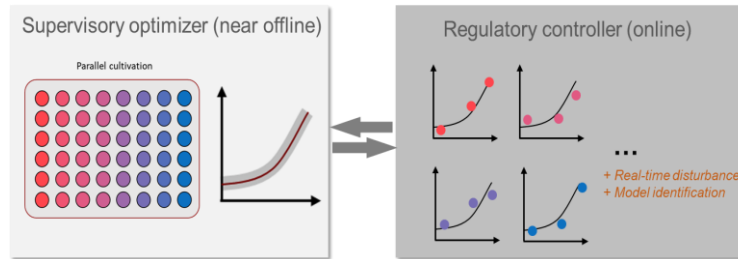
Niels Krausch

Kim et al. 2023. Model predictive control and moving horizon estimation for adaptive optimal bolus feeding in high-throughput cultivation of *E. coli*, Comp Chem Engin 172, 108-158, <https://doi.org/10.1016/j.compchemeng.2023.108158>.

MPC for Optimal Experimental Design

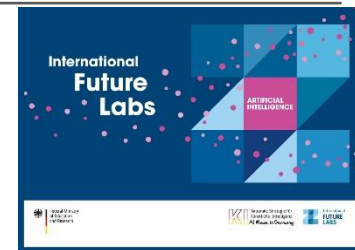


hierarchically decompose complex system



take home message

- we have today all the technologies required to change Research and Development in biotechnology and biopharma
- Data, Information, Knowledge, are the main bottle-neck for fast innovation
- The valorization of Knowledge is essential to motivate good data management practices
- Blockchain technologies can provide the transparency, traceability, and IP protection required to enable knowledge exchange between all R&D stakeholders.



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