MLExchange: bringing machine learning to scientific discovery

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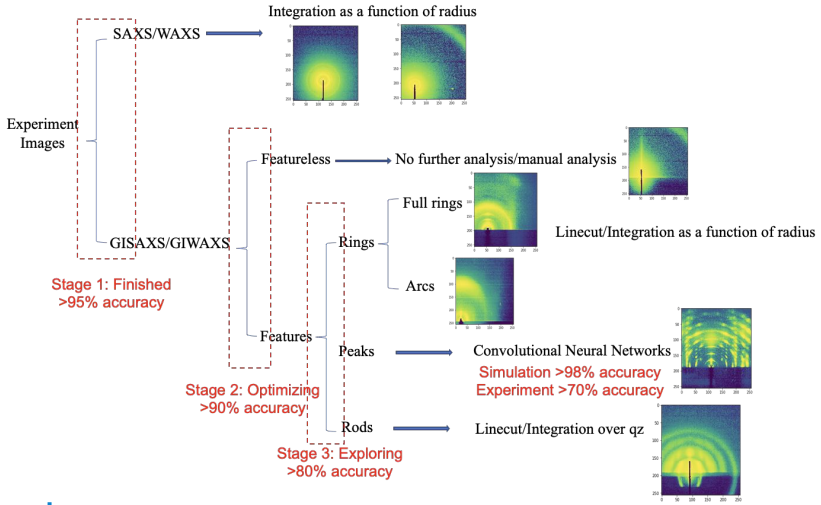
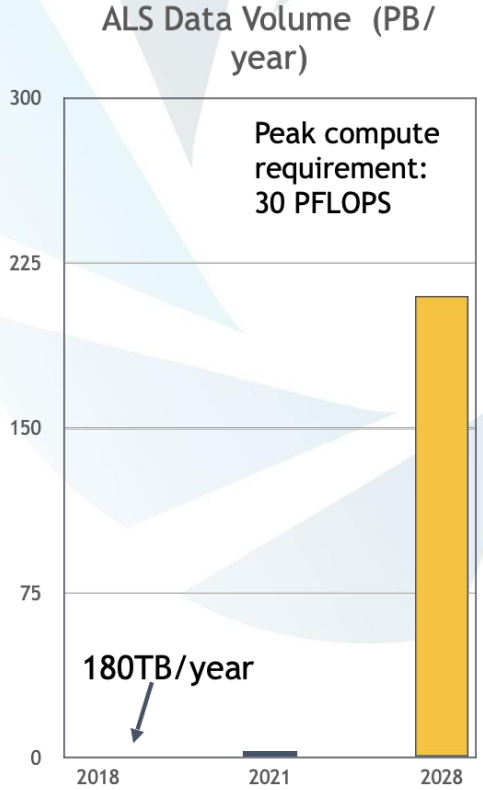
Challenges

Data challenges for beamline users

- Big amount of data, growing annually
- On-the-fly analysis dealing with various data types (spectra, image data, etc.)
- Interactive visualization tools

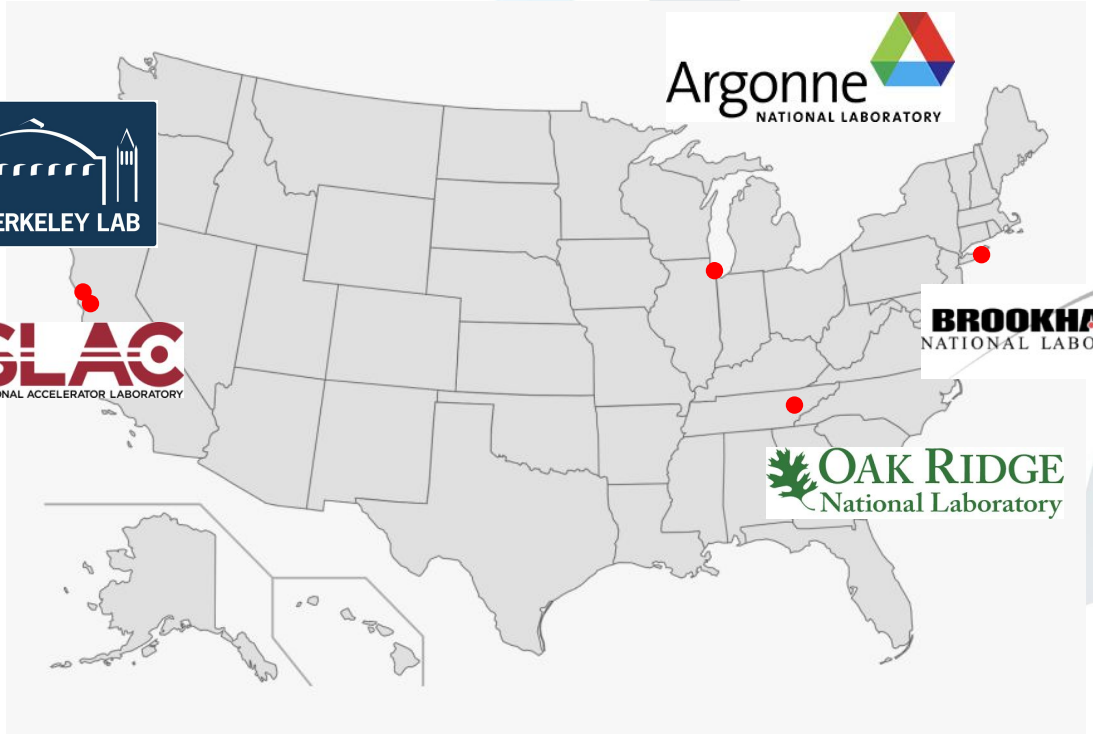
Machine learning tools can help!





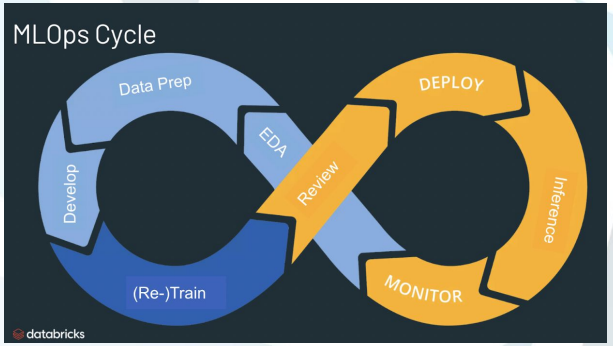
Challenges to use machine learning (ML)

- How to deploy and share ML workflows across DOE beamline facilities?



Challenges to use machine learning (ML)

- Many available ML tools require programmatic skills.
- Existing MLOps software:
  - not open-source (Weights & Biases)
  - do not have user system (MLflow)
  - do not have interactive interfaces customized for beamline users



General ML tool

Deep learning tools

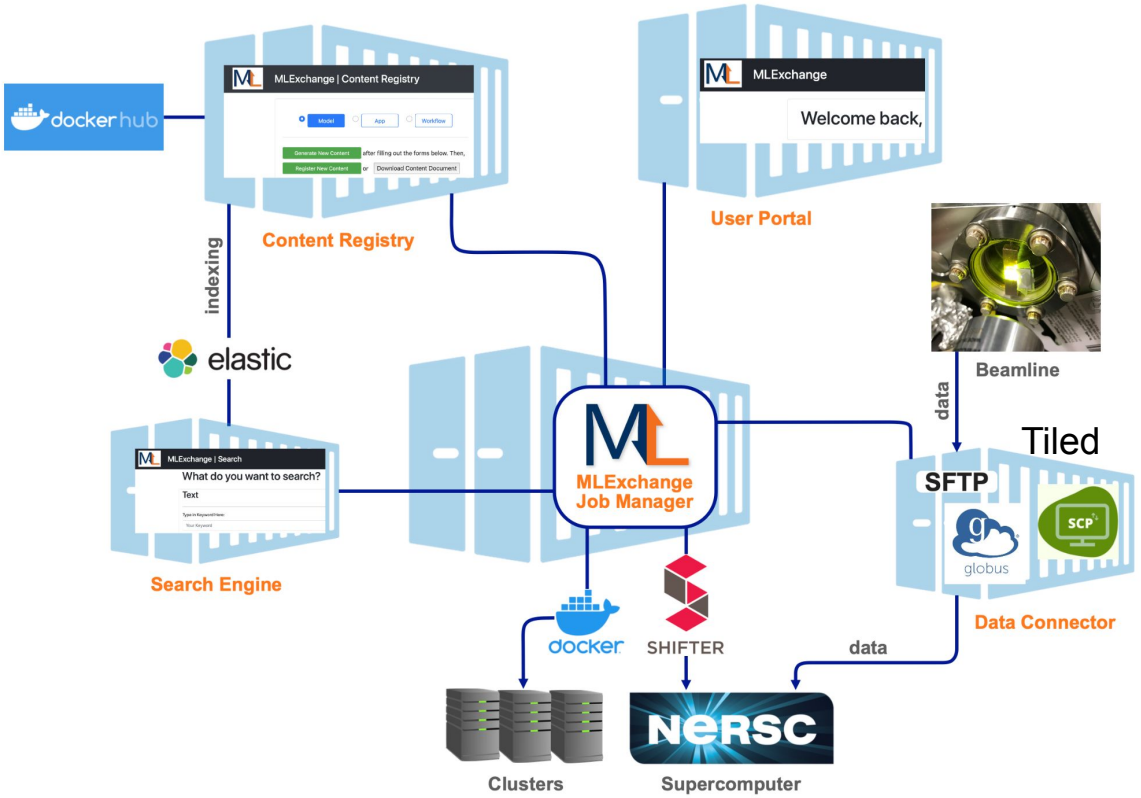
Data processing tools

Visualization tools

MLExchange platform

MLExchange architecture

- 5 major “containerized” components
- Communication through application programming interfaces (APIs)

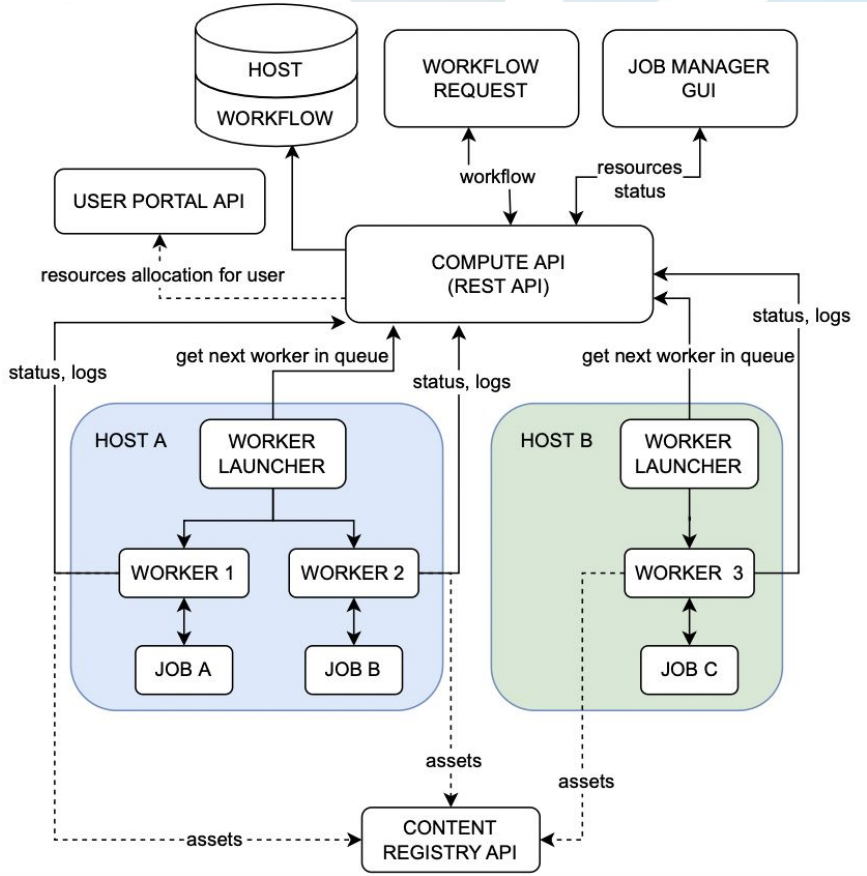


Major components

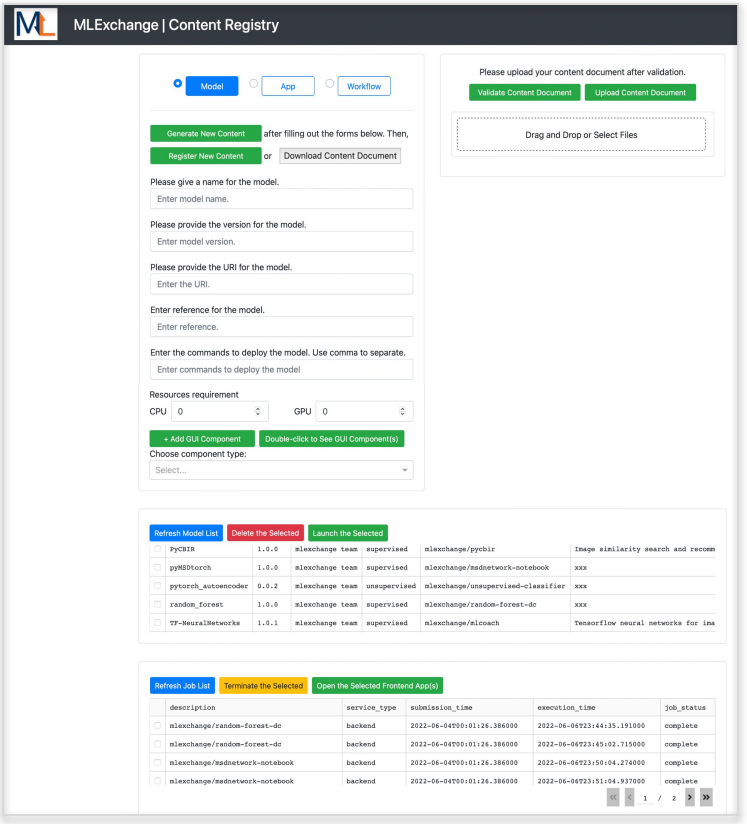
Job manager

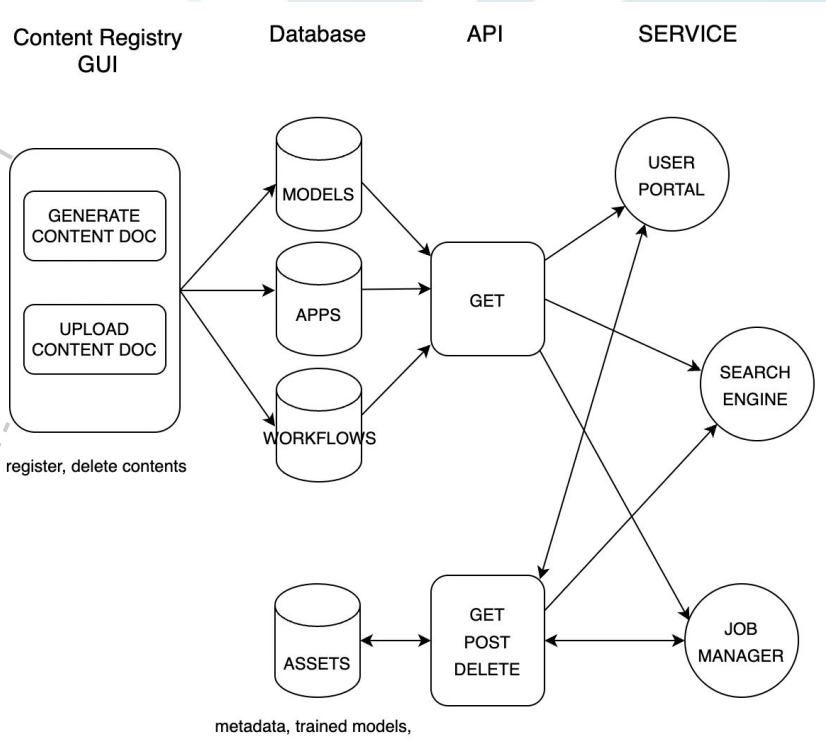
- A central job coordinator: a queue based on the timestamp and available computing resources.

Image source: Katerina Limpitsouni



Content registry





Content registry: **adaptive GUI components**

9 Dash component types

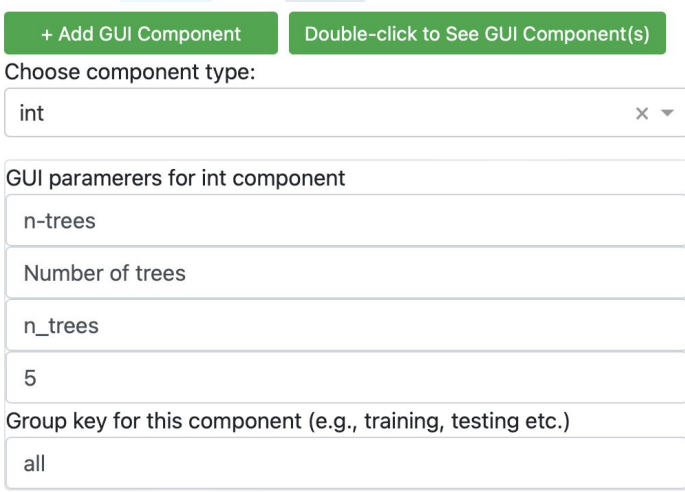
- 3 input forms (int float, str)
- Slider
- Dropdown window
- Radio items
- Boolean toggle switch
- Image
- Graph uploader

component id

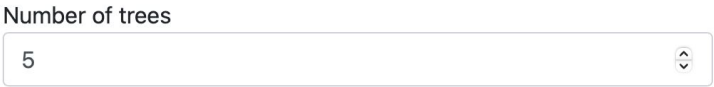
title (optional)

default value (optional)

group key (optional)

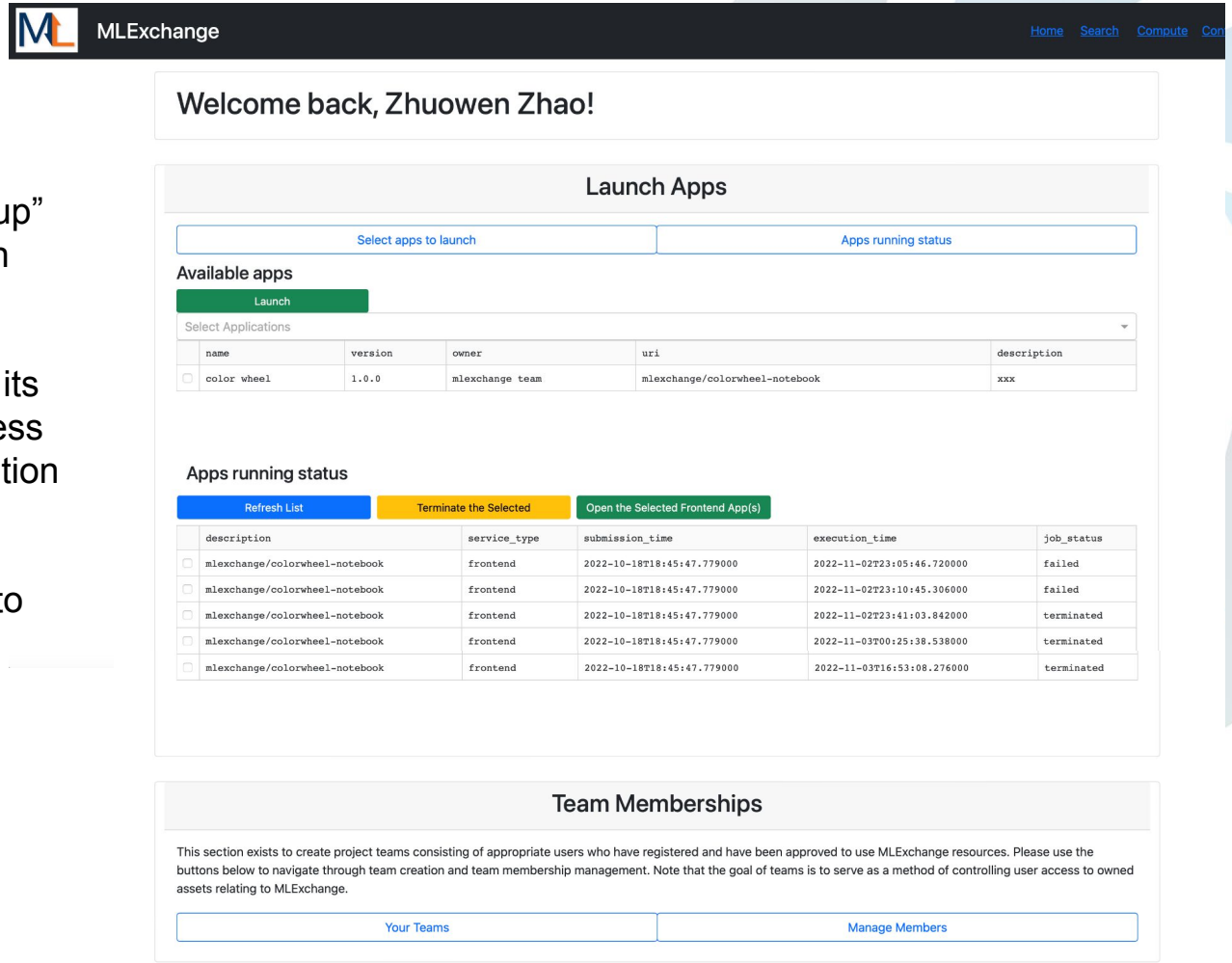


Automatically updates GUI components in frontend apps



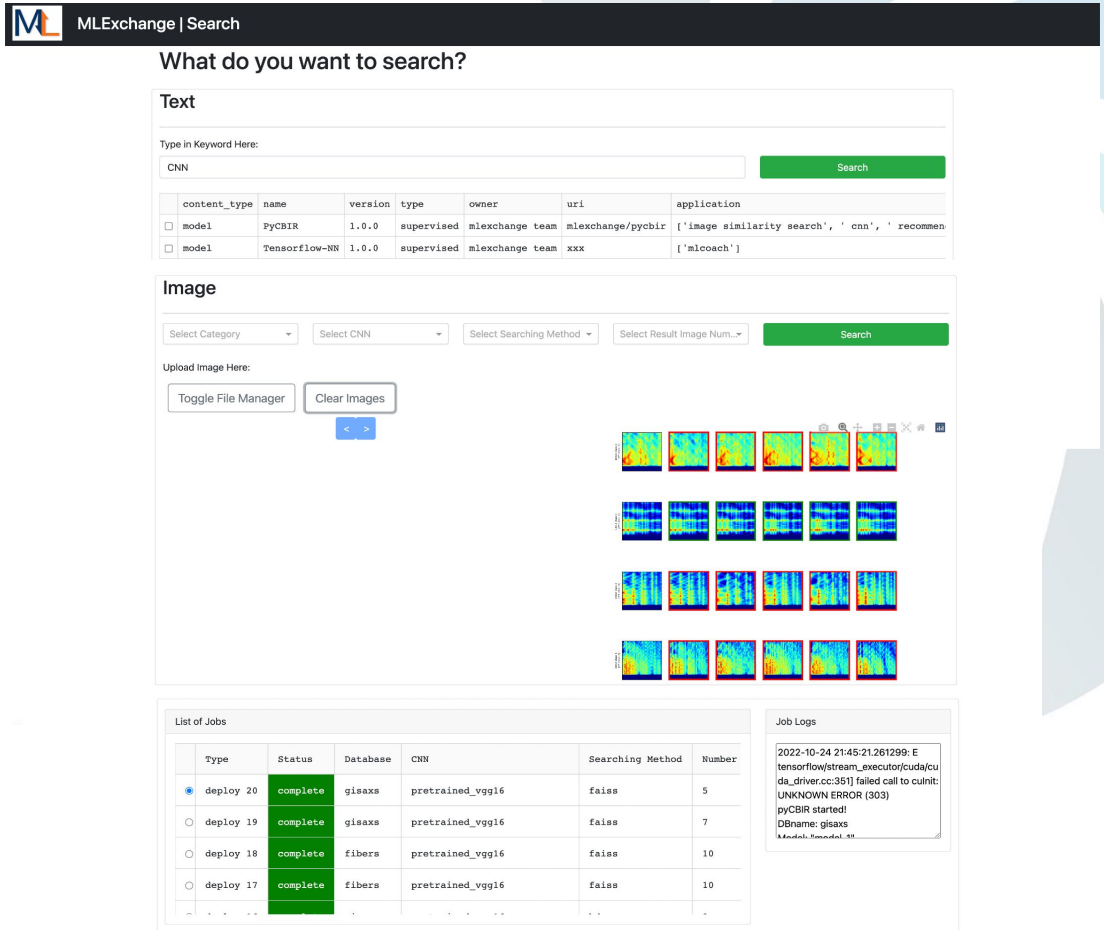
User portal

- Create “user-role-group” relationship in a graph database (neo4j)
- Insert the user id and its authority into the access token after authentication (Google)
- Launch/terminate/go to apps on behalf of individual user



Search

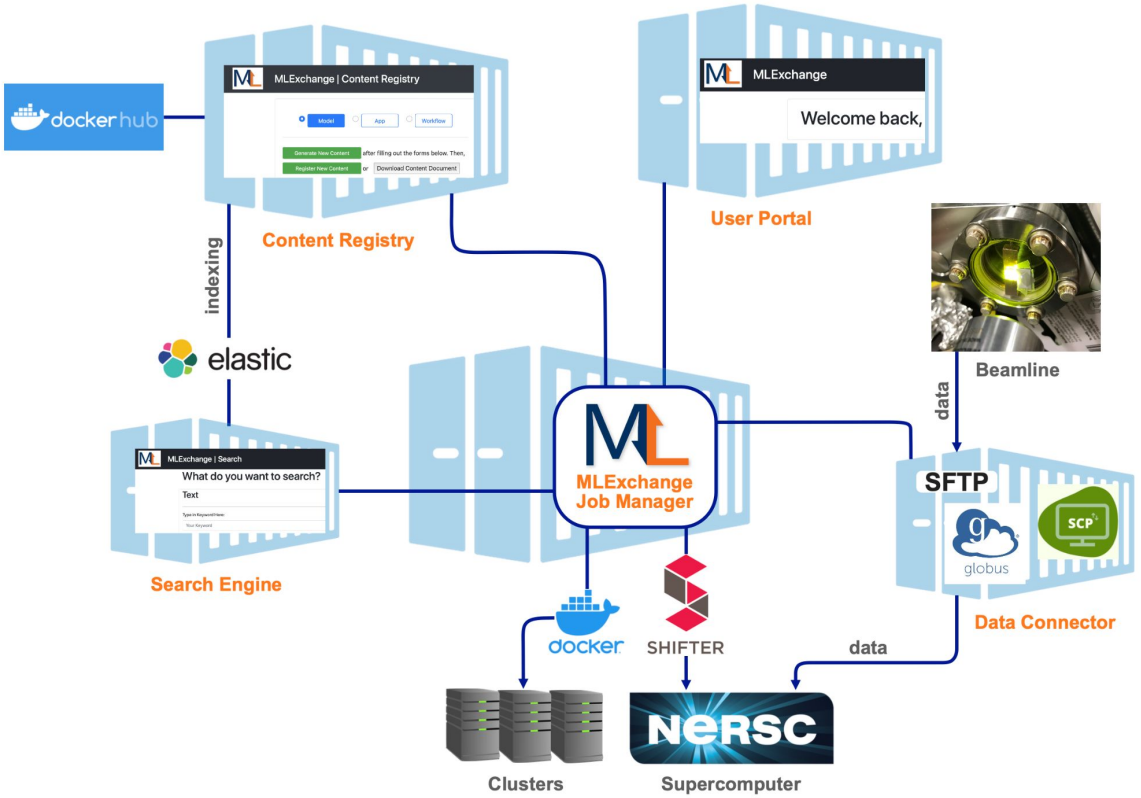
- Fast search for the contents stored in the content registry (based on user authority); it will evolve into a recommendation system.
- Search for similar images using pyCBIR[1] software



[1]pyCBIR is Python-based tool for content-based image retrieval (Araujo et.al. 2018)

Revisit MLExchange architecture

- Versatile deployment
- High modularity
- Scalability
- Easy accessibility



How-to live demo

How-to

Try MLExchange

GitHub: https://github.com/mlexchange/mlex

Docker Hub repository: https://hub.docker.com/u/mlexchange1

The official MLExchange portal: https://mlexchange.als.lbl.gov (Google authentication)

The development (beta) portal: https://mlexchangebeta.als.lbl.gov (Google authentication)

* Please note that Gmail account must be registered with both firstname and last name; o.w., you will see it keeps redirecting you back to the login page. The mlexchangebeta runs on our VM. We only have limited resources that support running max 6 (app) containers at the same time (automatically terminate in 5 mins).

How-to

Useful resources

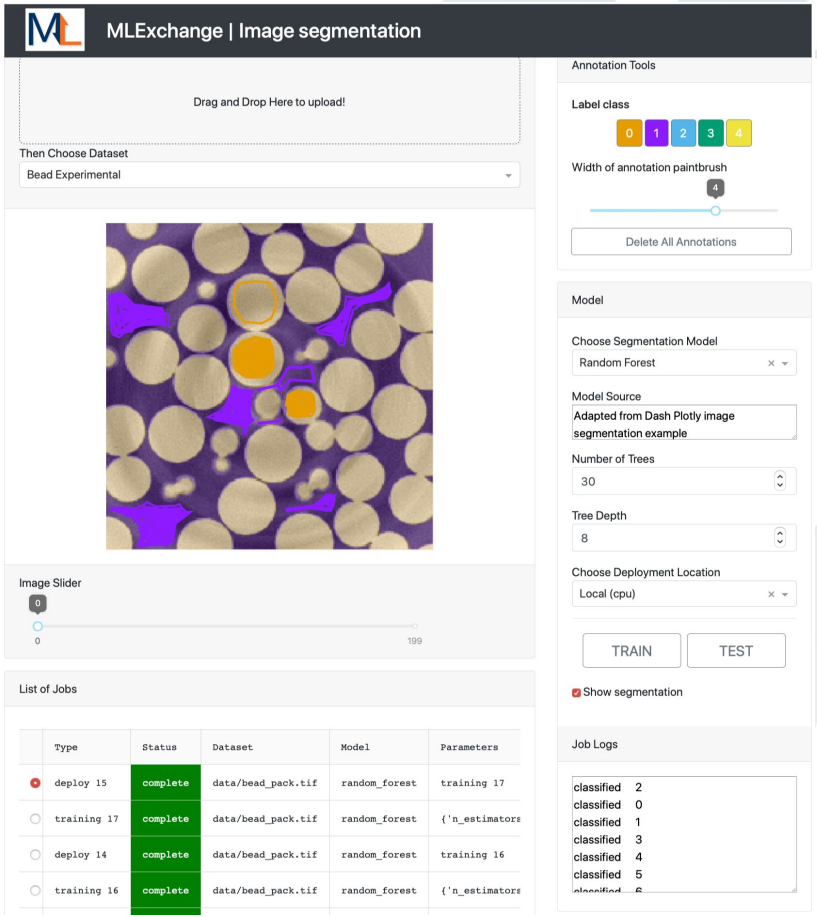
MLExchange documentation: https://docs.mlexchange.als.lbl.gov

MLExchange website: https://sites.google.com/lbl.gov/software-solutions-for-als/mlexchange

Use cases

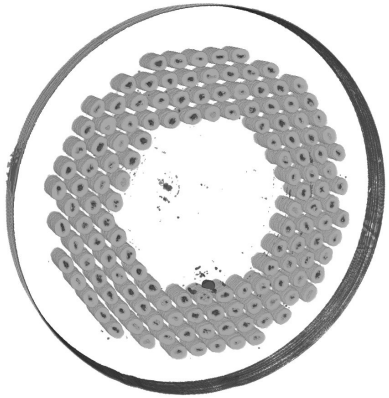
Use cases

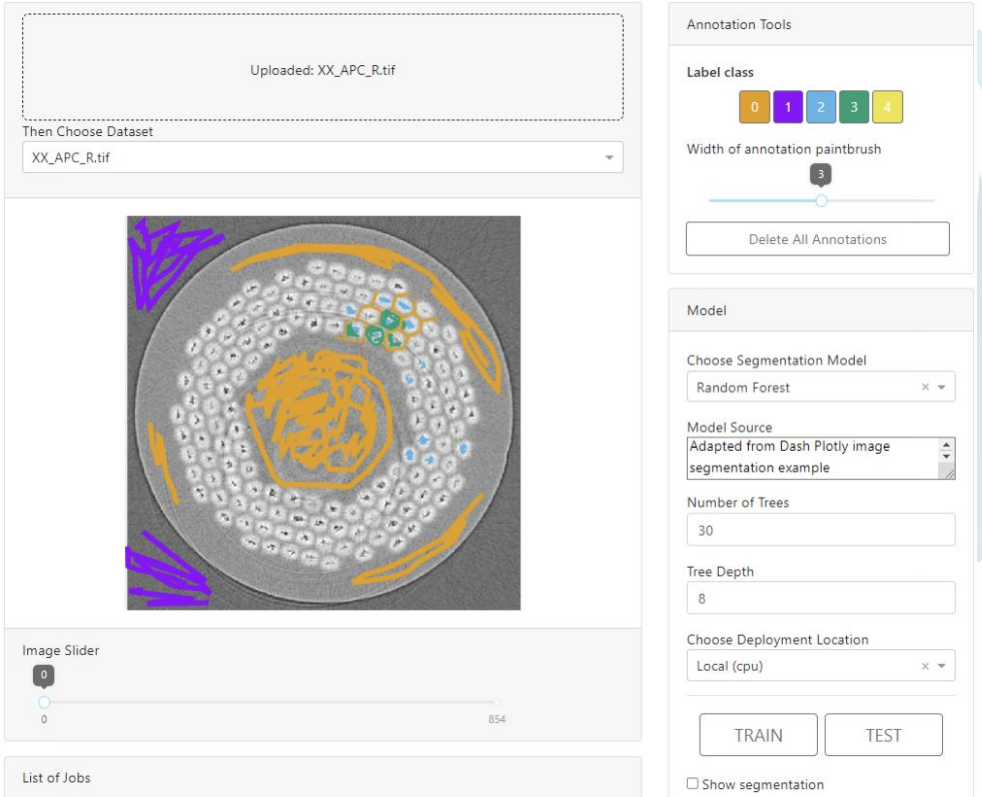
- Image segmentation: a “standalone” frontend app



APS tomography data

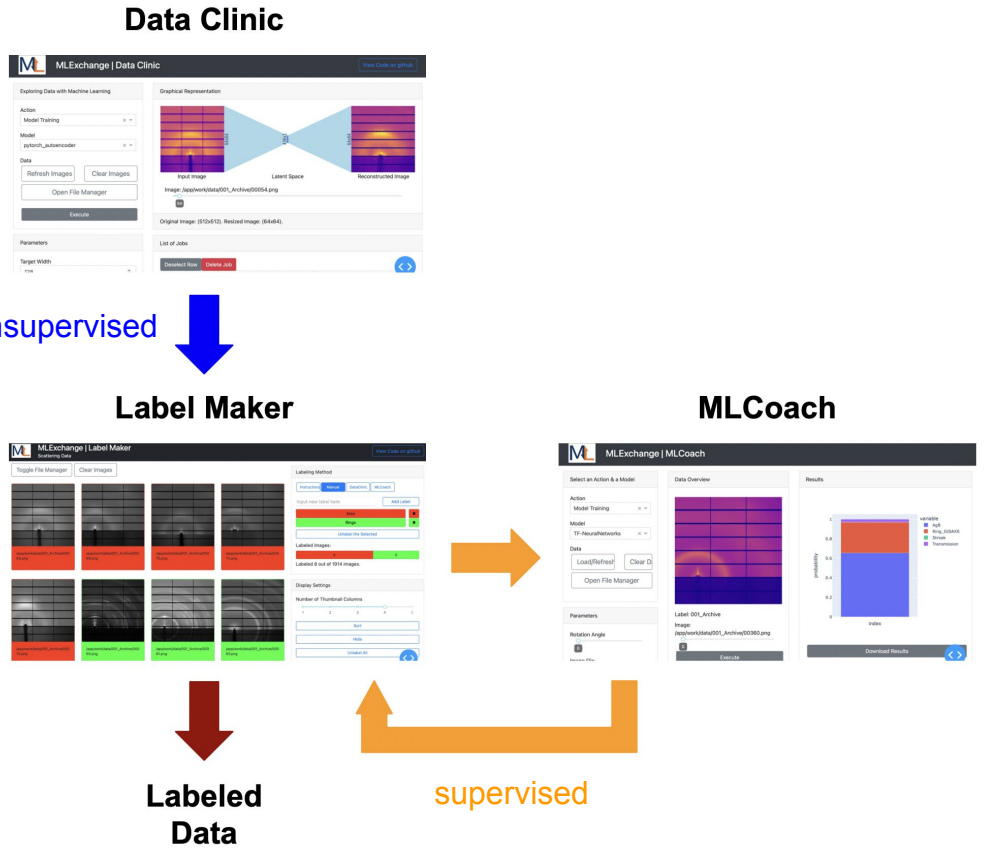
- Segmented area visualization (ImageJ 3D viewer) by Jean-Francois Croteau





Use cases

- Image labeling pipeline: a combination of multiple frontend apps



Thank you !

Q & A

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