

MLExchange — A web-based platform enabling exchangeable machine learning workflows

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Abstract—Machine learning (ML) algorithms are showing a growing trend in helping the scientific communities across different disciplines and institutions to address large and diverse data problems. However, many available ML tools are programmatically demanding and computationally costly. The MLExchange project aims to build a collaborative platform equipped with enabling tools that allow scientists and facility users who do not have a profound ML background to use ML and computational resources in scientific discovery. At the high level, we are targeting a full user experience where managing and exchanging ML algorithms, workflows, and data are readily available through web applications. So far, we have built four major components, i.e., the *central* job manager, the *centralized* content registry, user portal, and search engine, and successfully deployed these components on a testing server.

Since each component is an independent container, the whole platform or its individual service(s) can be easily deployed at servers of different scales, ranging from a laptop (usually a single user) to high performance clusters (HPC) accessed (simultaneously) by many users. Thus, MLExchange renders flexible using scenarios—users could either access the services and resources from a remote server or run the whole platform or its individual service(s) within their local network.

Index Terms—machine learning, platform, exchangeable workflows, data pipelines, versatile deployment

I. INTRODUCTION

The scientific user facilities (SUF) of the Department of Energy (DOE) are capable of producing over 10 petabytes of experimental and simulated data per year, making them

among the biggest data producers in the world [1, 2]. The data span multidisciplinary sciences covering multi-faceted and complex interactions that require domain expertise to decipher intricate relationships within natural phenomena. Coordinating these complex data analyses is much needed because it can not only lead to new knowledge but also aid in building and optimizing the use of experimental facilities. Fortunately, new advances in scientific machine learning (ML) offer an opportunity to leverage the commonalities, scientific insights, and collected experience of the larger scientific user facility community. However, a lot of available ML tools require users to have programmatic coding experience and a considerably profound ML background. To meet the ever-increasing need for domain scientists who do not necessarily have a deep ML background to use fast-growing ML algorithms and to facilitate the ML ecosystem among SUF, we are building a user-friendly platform called *MLExchange* to allow ML algorithms and applications to be readily exchanged and deployed across the DOE facilities. As such, MLExchange is designed to have high deployability for each granular service, allowing it to accommodate various deployment situations. Furthermore, the platform has high modularity, scalability, and easy accessibility.

Versatile Deployment Every MLExchange service (a platform component, an algorithm, an frontend application, etc.) is a container [3] that contains the required environment to run

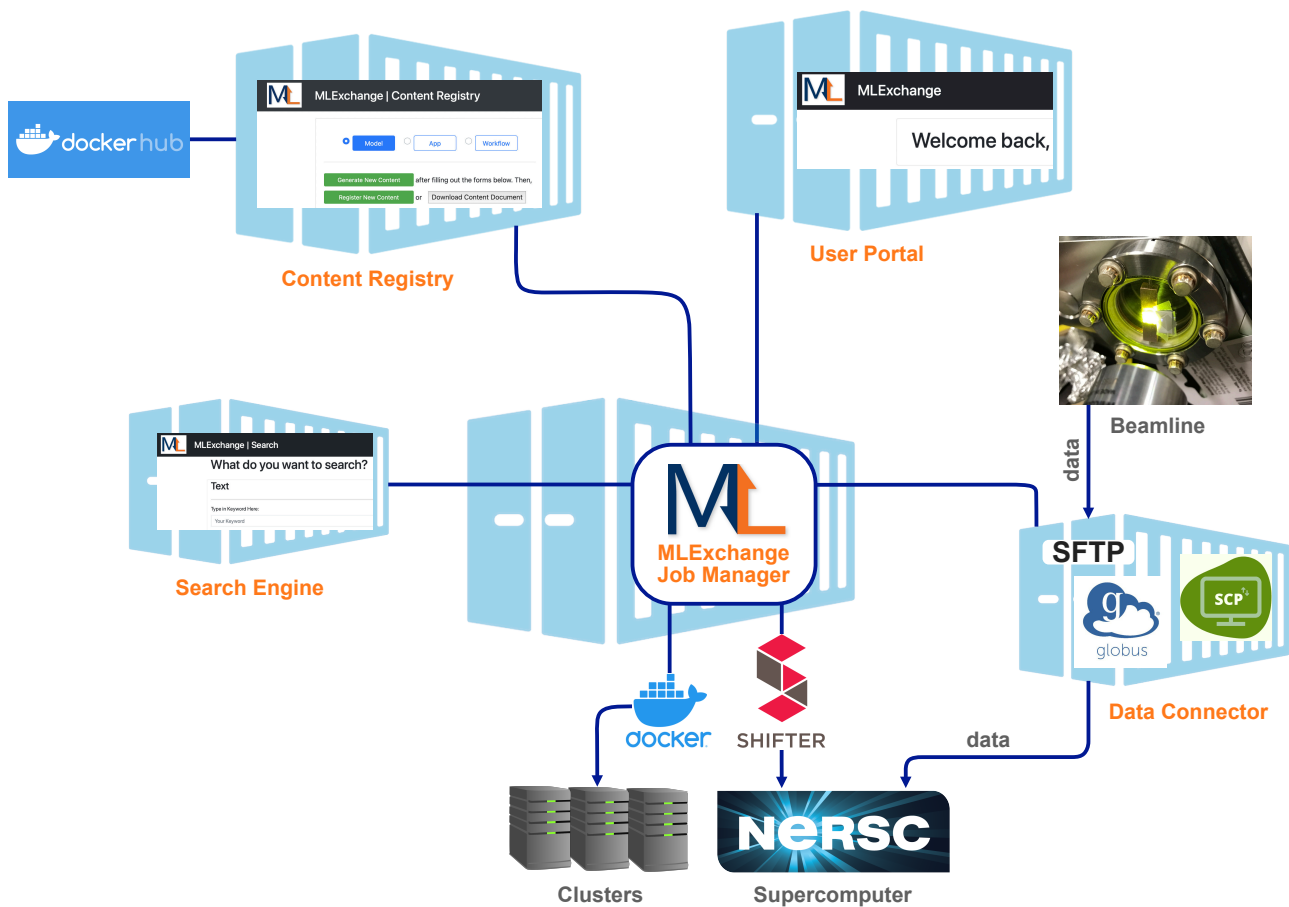


Fig. 1. MLEExchange architecture

independently across different hardware.¹ This enables MLEExchange services to be easily deployed at different locations, such as a laptop, a workstation at a beamline station, and high performance clusters (HPC). For example, the official MLEExchange platform is deployed at Vaughan (located at the Berkeley Lab), whose resources are open to DOE facility users.² Nevertheless, users also have the option to deploy the whole platform or its individual services within their internal networks and not share their resources.

Modularity MLEExchange can construct ML workflows of any complexity. An MLEExchange workflow is a combination of frontend apps (e.g., a Dash app) and/or backend jobs (e.g., a ML algorithm). For instance, a typical workflow would consist of a few frontend apps to form an analysis, and each app could use a list of available backend algorithms. With the content registry, users can ingest these pre-defined workflows, new

algorithms, and apps into the platform, thus populating use cases (examples are discussed in Section III).

Scalability There are two aspects of MLEExchange scalability. First, MLEExchange is designed to accommodate a large user base. Its user portal is responsible for registering new users, authenticating user identity, and authorizing access to services and resources. In terms of computing, the job manager is designed to handle multi-job situations, e.g., allocating computational resources for individual jobs. Second, because of the high modularity, the user community can scale up MLEExchange applications and use cases.

Accessibility MLEExchange is a web-based platform. Users can access its official version through <https://mlexchange.als.lbl.gov>.

¹MLEExchange currently uses Docker containers that run on both ARM and AMD architectures. Other containers, such as Shifter containers, will be included in the next version.

²A NGINX proxy system is adopted to enable secure access to MLEExchange frontend services on Vaughan.

With the above design features, we expect MLEExchange to cater to the needs of beamline scientists and facility users under various situations. Moreover, other entities or companies may also find MLEExchange a helpful platform.

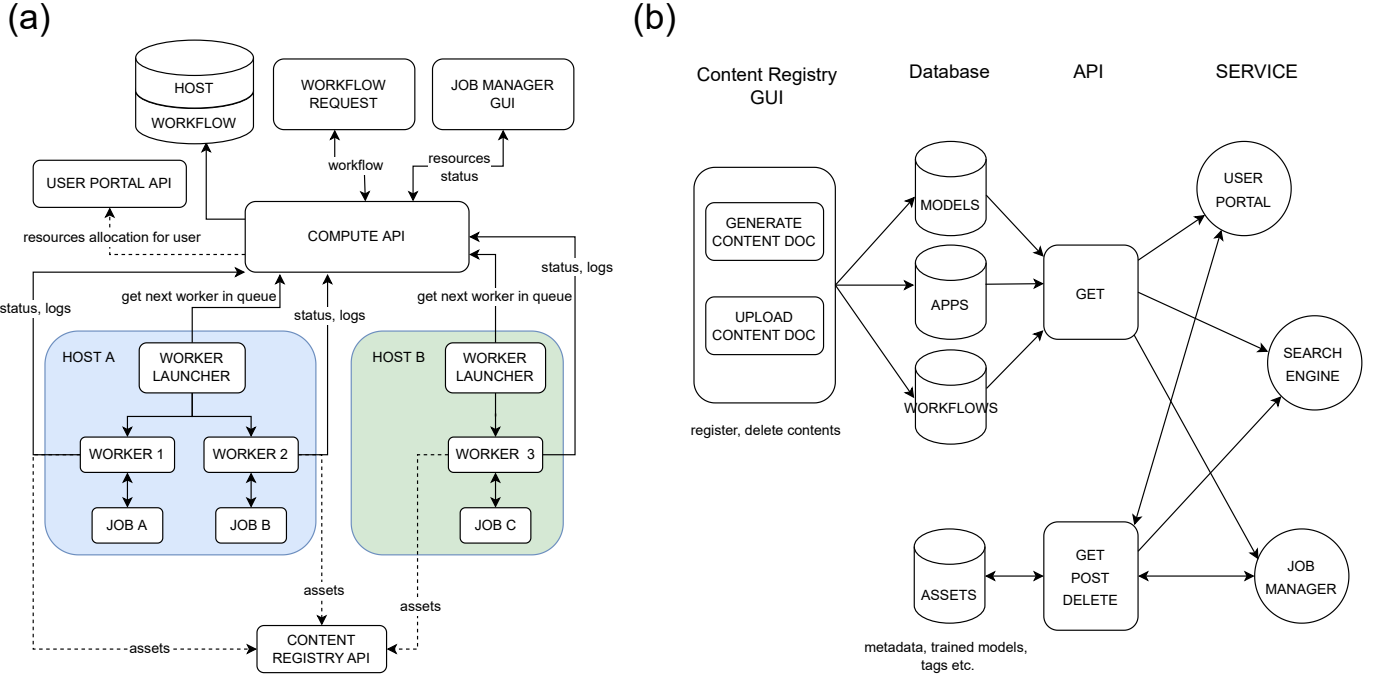


Fig. 2. (a) Diagram of the job manager, where the solid lines represent the current implementation of this component, and the dashed lines correspond to new features in the next release; (b) Schematics of the content registry and its APIs. Arrow pointing right means the operation can only fetch content(s) from the upstream, whereas pointing left denotes altering content(s) in the upstream.

II. ARCHITECTURE

As is shown in Fig. 1, the platform has 5 major components: the *central* job manager, the *centralized* content registry, user portal, and search engine, and the data connector. The job manager is expected to be deployed at different servers to leverage various computing resources (“central” at the server level). While the other components remain centralized even though users can also have a local copy of them if needed.

In MLExchange, an entity is treated as either a job or content. A job is a running program using computing resources (CPUs and GPUs). A “static” content, e.g., a (learned or unlearned) ML algorithm, a Dash frontend, a computing resource, or metadata produced by a finished job, is stored and managed by the content registry.³ Whereas a “dynamic” content associated with a running job, e.g., a set of input parameters for a running model or job logs, is stored and managed by the job manager. Note that, throughout the paper, it has the static context by default when referring to a content. The search engine offers content searching and ranking services, and the data connector is responsible for securely transferring MLExchange contents to different locations. The user portal will authorize access to the above services, then jobs from those services will be carried out by the job manager on behalf of the individual user.

All these components can communicate through application programming interfaces (API) endpoints, each using a unique resource locator (URL).

³User information and their hierarchical relationships are stored in the user portal graph database.

A. Job manager

The job manager is a central job scheduler that coordinates job executions according to the availability of computing resources and services requested by the other MLExchange components. As is shown Fig. 2 (a), the job manager currently consists of an API service (compute API), a database, a worker launcher per host, and the job manager GUI.

The job manager executes workflows at the top of the hierarchy. A workflow is constructed as a list of jobs with their corresponding dependencies, a pre-defined set of computing resources (CPU/GPU), and the number of workers. The workflow execution involves allocating compute resources to the workers, where the compute API uses a supply-constrained definition setup to schedule workers through constraint programming and Satisfiability (cp-SAT) methods [4].

The compute API distributes workers among worker launchers (hosts) when a workflow is received. Then, the worker launchers will launch worker containers to execute workflow jobs in the background. The worker launchers periodically communicate with the compute API looking for compute resources to deploy the next workers in the queue. Each worker runs their assigned jobs—one at a time—according to their dependency setup and reports their current status, logs, and newly-generated assets back to the compute API. Once a worker completes its job list, it will terminate itself and release the resources back to the host.

B. Content registry

The content registry consists of a GUI, a centralized database, and a set of APIs to manage the ingestion, removal, and pulling of these contents, see Fig. 2 (b). The database currently stores four types of contents, i.e., models (algorithms), applications (apps), workflows, and assets (metadata such as service parameters). Content(s) (all types) can be added, deleted, and retrieved to/from the content registry database through API calls. In addition, a content of the model/app/workflow type can also be registered using the GUI by either filling out the required forms (also generates the content document) or uploading an existing content document (JSON file). The GUI displays the available models/apps/workflows in a table where users can navigate and delete contents as well as submit services (execute or stop containers) of the selected contents to the job manager.

Note that the content registry does not store the actual content. Instead, it stores the specifications of the content and a pointer (URL) to the place where the content is actually stored.

C. User portal

The user portal provides user management services at both the administrator and participant levels. From a generic perspective, it is responsible for user authentication and authorization of the MLEExchange services. We use attribute-based access control (ABAC) [5] implemented over a Neo4J graph database to enable flexible yet powerful formalization of access policies across a variety of access management cases. Using a graph database that we query with Cypher [6], we can efficiently query and analyze connected data over a set of complex policies to enforce hierarchical access to MLEExchange content registry and user-owned assets.⁴ Management of owned assets can be executed at a participant (single user), owner-defined team (group of users), or community-level (all users).

D. Search engine and data connector

Two other essential MLEExchange services are content searching and ranking through the search engine and secure data transfer via the data connector. The search engine uses Elasticsearch to provide fast and high-volume content searching answers. It also contains a reverse image searching pipeline [7] that allows users to search for similar images based on deep neural network algorithms. The data connector is currently under development. It will contain a GUI where users would have a collection of secure data transfer technologies to use, such as Secure File Transfer Protocol (SFTP), Secure Copy Protocol (SCP), and Globus.

III. USE CASES

A. Image segmentation

We adapted the image segmentation workflow from Dash Enterprise App Gallery [8, 9] and successfully integrated it

⁴Common examples of user-owned assets include but are not limited to trained ML models, workflows, and privately-owned computing resources.

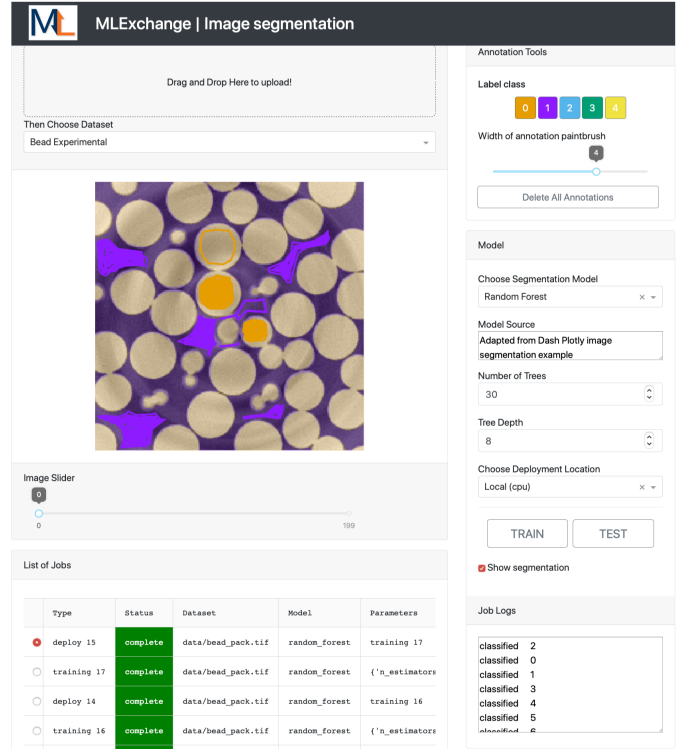


Fig. 3. MLEExchange image segmentation user interface. It shows the segmentation results from using the Random Forest with an overlay of label shapes.

into the MLEExchange platform. In addition to interactively uploading new datasets, more user-friendly workflow features are added to the application.

General Procedures Users need to register a new ML algorithm in the content registry before using it from the user interface. The interface supports labeling, training models, and segmenting images, see Fig. 3. All models follow a TRAIN-TEST procedure: a learned model is saved in the TRAIN step and will be used to segment the full image stack in the TEST step. Although labeling is not needed for an unsupervised model (K-means) in the TRAIN step, users can select a portion of the images as inputs for the unsupervised learning in this step. In the Show Segmentation mode, pixels will be colored according to the corresponding label class.

ML Models Currently, three ML algorithms are available, i.e., Random Forest [8], K-means clustering [10], and Mixed-Scale Dense Convolutional Neural Networks (MSDNet) [11–13].

Adaptive GUI Components The model parameter layouts are automatically generated and updated when selecting a different model. The keywords to describe these Dash components are pre-defined in the content registry. A code takes these keywords and updates the children property of the respective Dash components such that the layouts in the Dash user interface are automatically refreshed. This is a key MLEExchange feature as it allows users to ingest new algorithms without the need to modify the source code of their frontend applications.

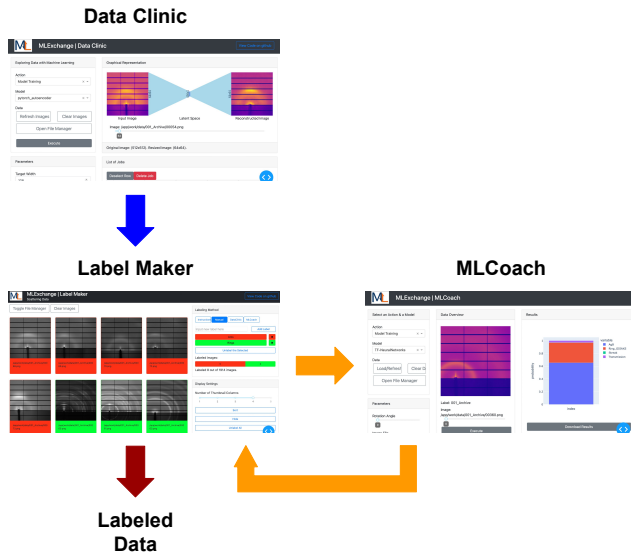


Fig. 4. MLEXchange image labeling pipelines: (1) unguided manual labeling through Label Maker, and ML-assisted labeling through (2) Dataclinic (self-supervised) → Label Maker; (3) Label Maker (manual labeling) → MLCoach (supervised) → Label Maker (auto labeling)

Workflow Execution In this use case, a workflow only has one job per user request (TRAIN or TEST).

B. Image labeling

In contrast to the single application case (image segmentation in Section III-A), the image labeling pipelines streamline the labeling process for large datasets with three “standalone” frontend applications, i.e., Label Maker, Data Clinic, and MLCoach, see Fig. 4. Label Maker has an integrated interface for manual labeling and ML-assisted labeling steps using the results from the other two applications.

Self-supervised Learning Approach Data Clinic provides the similarity score (the Euclidean distance between two latent vectors) for a given target image against each image within the dataset through a well-trained autoencoder. Label Maker exploits such results by arranging the images from the most similar to the least alike, where users can proceed to label them in batches.

Supervised Learning Approach MLCoach trains neural networks with a set of previously labeled images to classify the whole dataset, where the classifier’s output is the prediction probability per class. Then, Label Maker can automatically label each image on condition that its predicted probability exceeds a user-defined threshold for a specific class (e.g., 50 %).

Workflow Execution The image labeling pipelines have three standalone frontend applications that can be launched in parallel or any order. For each application, a workflow works the same way as the image segmentation application.

IV. SUMMARY AND OUTLOOK

MLEXchange is a web-based platform that manages the full life cycle of ML tools which is accessible and easy to use for beamline scientists. So far, we have built four major components, i.e., the central job manager, the centralized content registry, the user portal, and the search engine. The last major component, the data connector, is under development. Additionally, we have implemented an assortment of web applications for scientific analysis of multimodal datasets, such as grain/pattern orientation detection, latent space exploration, data labeling, peak detection, inpainting detector gaps in X-ray scattering [14], and artifact identification [15].

Future development of the MLEXchange platform will be focused on optimizing user experience (completing the data pipelines, supporting more container technologies, etc.) and including more use cases for scientific research.

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CODE AVAILABILITY

The MLEXchange platform source codes can be found at <https://github.com/mlexchange>.

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