AI Intro Basics #5

MLflow
an open-source platform for managing the machine learning lifecycle

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E-AI Basic Tutorials

Tutorial E-AI Basics 4: January Wednesday 22, 2025, 11-12 CET
"MLOps" - Machine Learning Operations
4.1 Overview (20') [RP]
4.2 MLOps in relation to traditional Weather forecasting (20') [MJ]
4.3 Road to MLOps (20’) [DN]

5.1

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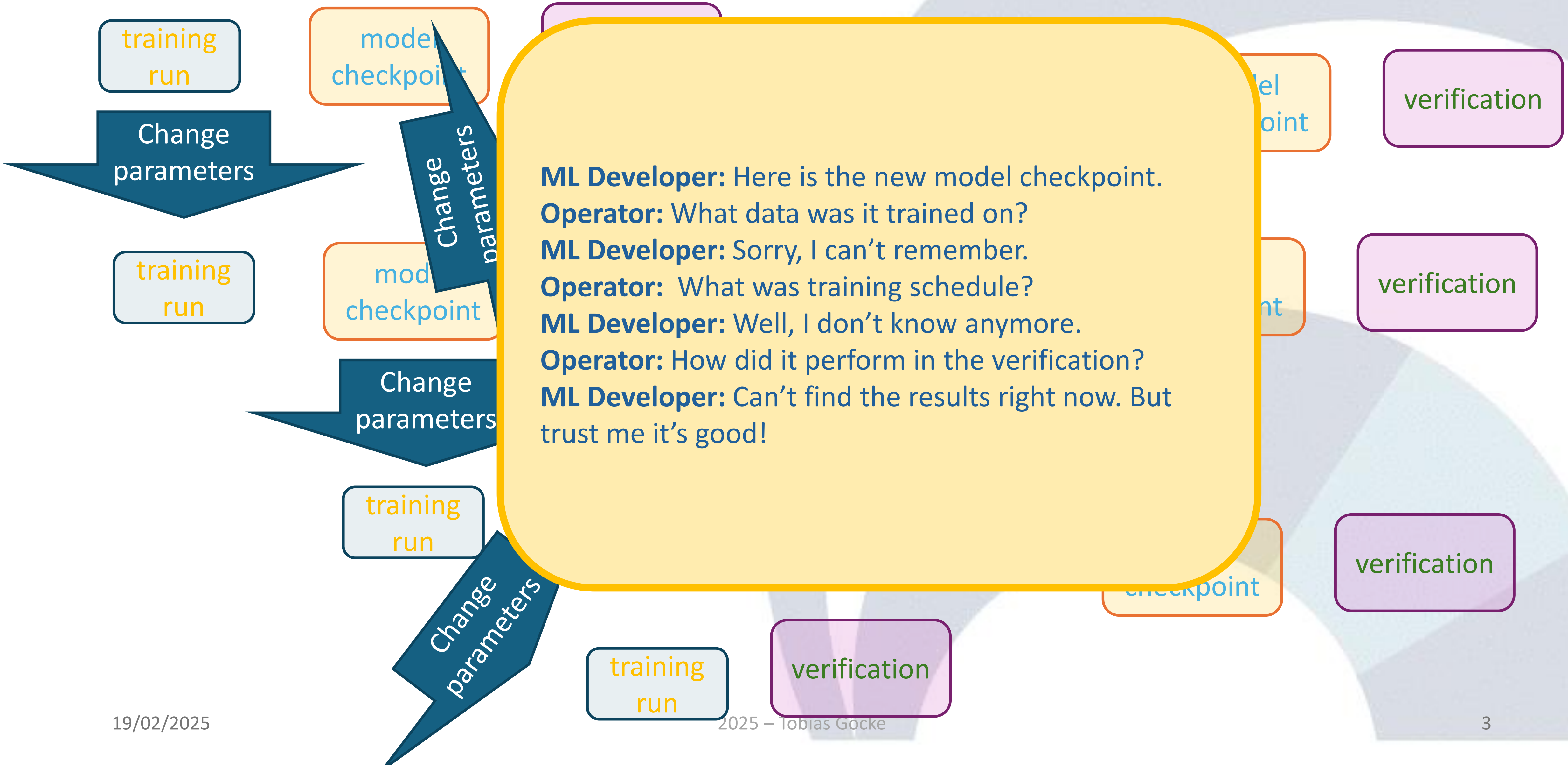
Why experiment tracking?



ML Developer: Here is the new model checkpoint.
Operator: What data was it trained on?
ML Developer: Sorry, I can’t remember.
Operator: What was training schedule?
ML Developer: Well, I don’t know anymore.
Operator: How did it perform in the verification?
ML Developer: Can’t find the results right now. But trust me it’s good!

Experiment tracking options (subjective comparison after short research)

mlflow™

- Open source
- User-friendly
- Well documented
- Configurable
- Flexible
- Integrates with different environment (pytorch)
- Can set up a local stand alone server easily

TensorBoard

- Integrates especially well with tensorflow
- Not ideal for large scale projects?

Weights & Biases

- Hosted service
- Has to be paid

Experiment tracking with MlFlow

- Place where to log and organize training runs
  - Experiments, each consisting of various runs
- Reproducibility
  - Log software versions, configs, model checkpoints
- Live monitoring
  - Validation metrics, system metrics, plots, etc
- Powerful tools to compare runs
  - Diffs in parameters
  - Multi run loss plots
  - Understand hyper parameters
- Different modes
  - local
  - Stand-alone server
  - Web-server

Quick-start mlflow

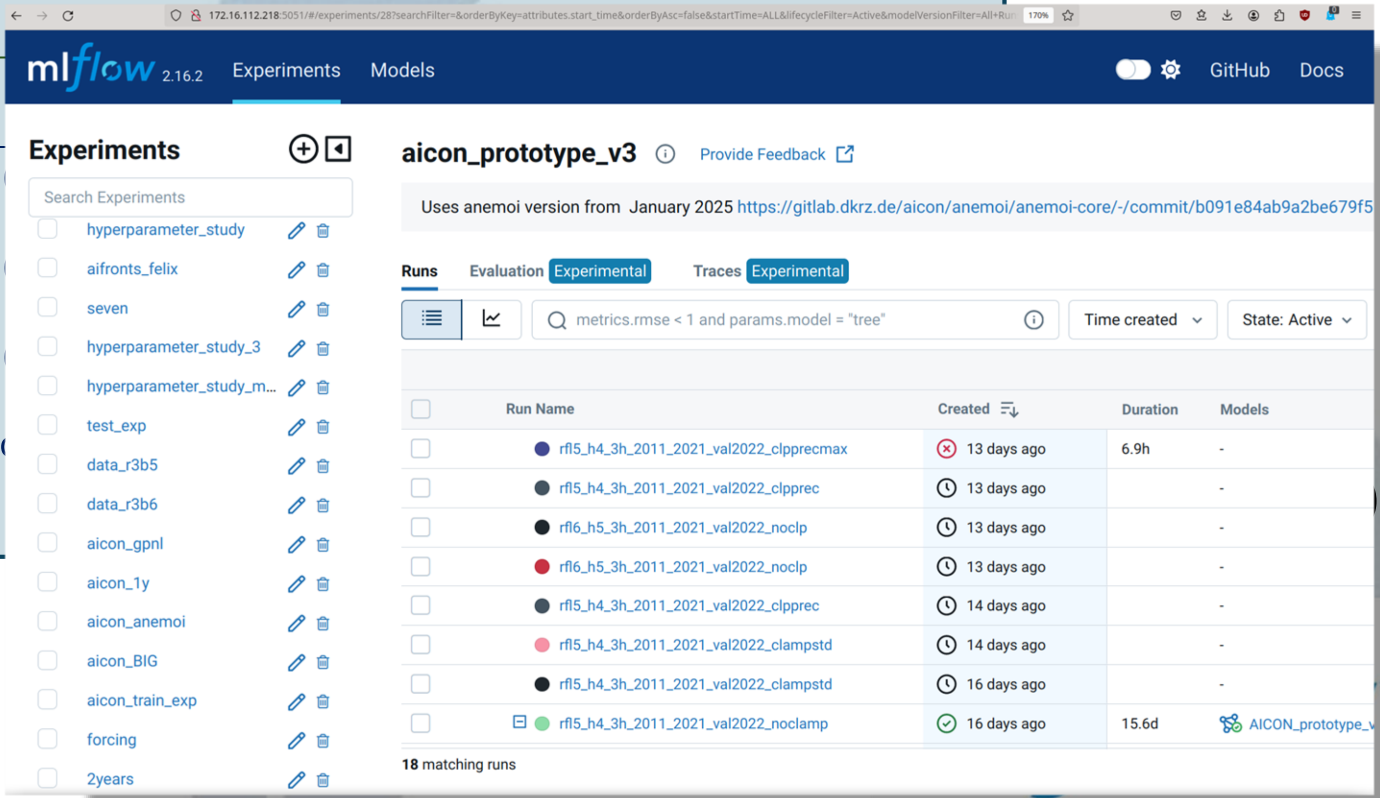
- Install

```
pip install mlflow
```

(virtual python environment)

- Log

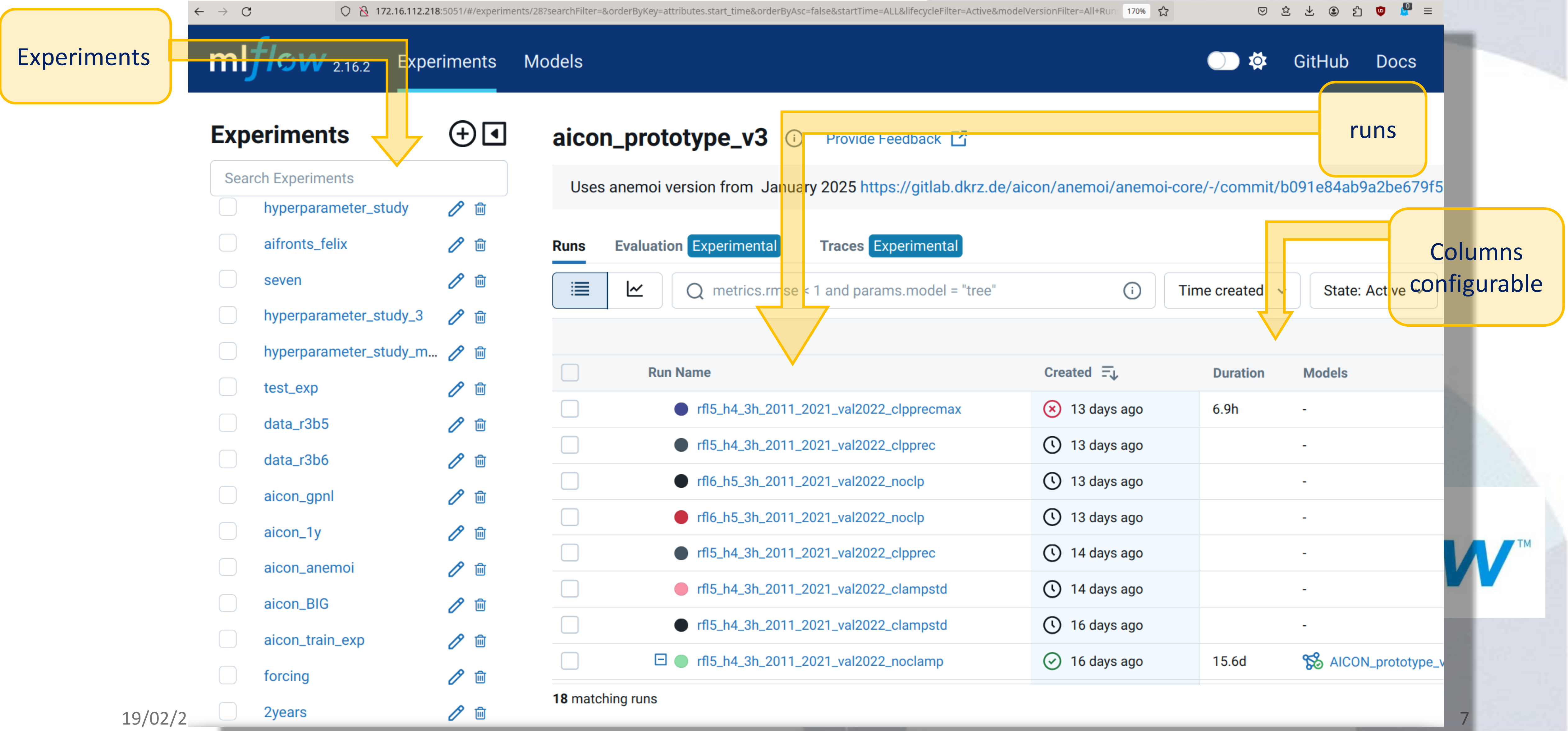
```
import mlflow
mlflow.set_experiment("my_
[…]
with mlflow.start_run(run_
        mlflow.log_params
        […]
        mlflow.log_metric
        […]
        mlflow.log_figure
        […]
        mlflow.log_artifa
```



- View

```
mlflow ui
```

Mlflow web user interface



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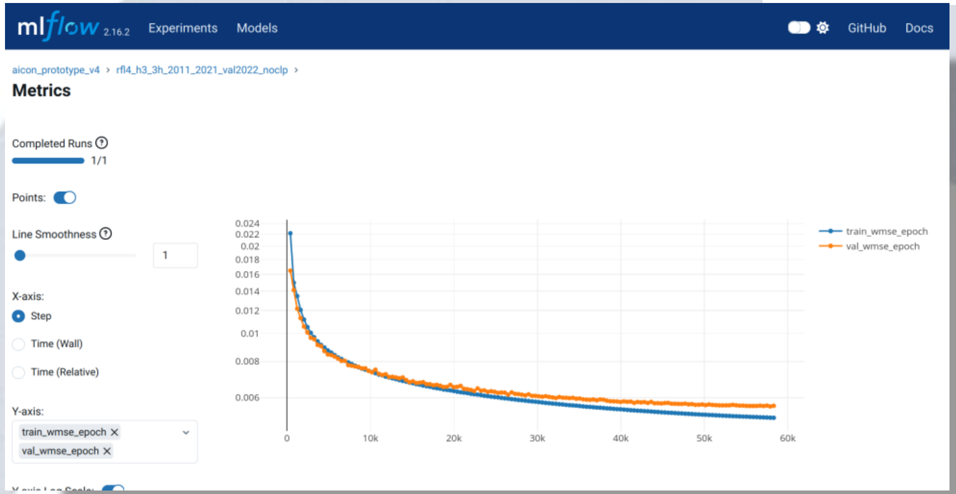
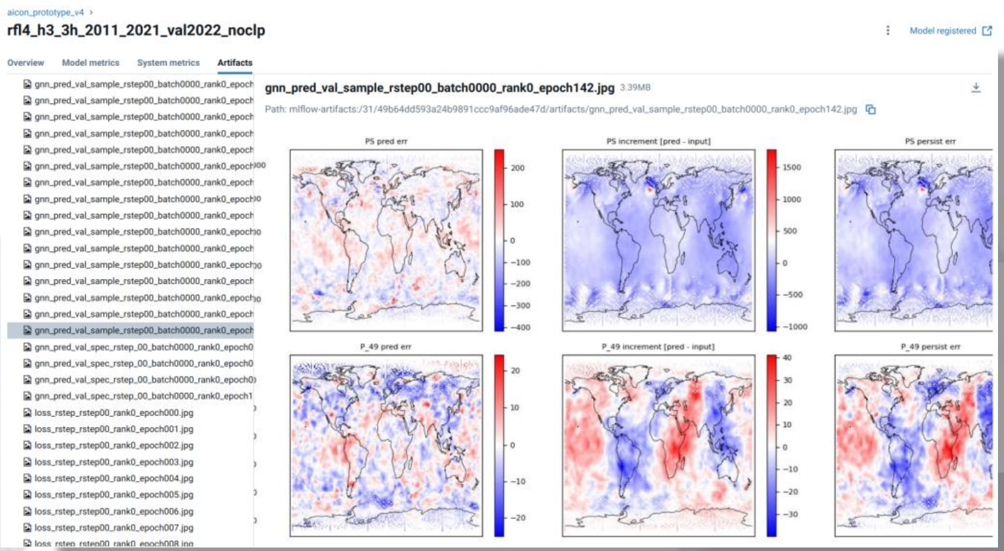
Mlflow web user interface

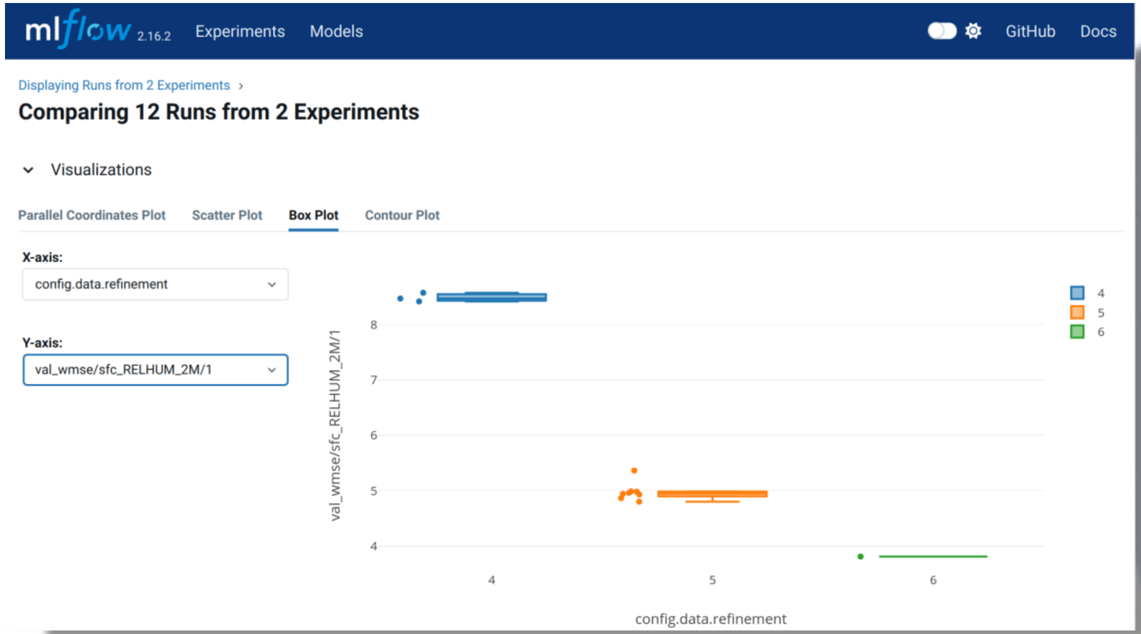
- Plot various metrics
- Compare different runs
- Log plots
- Compare parameter settings
- Summary plots for hyper parameter studies
- Compare across different experiments

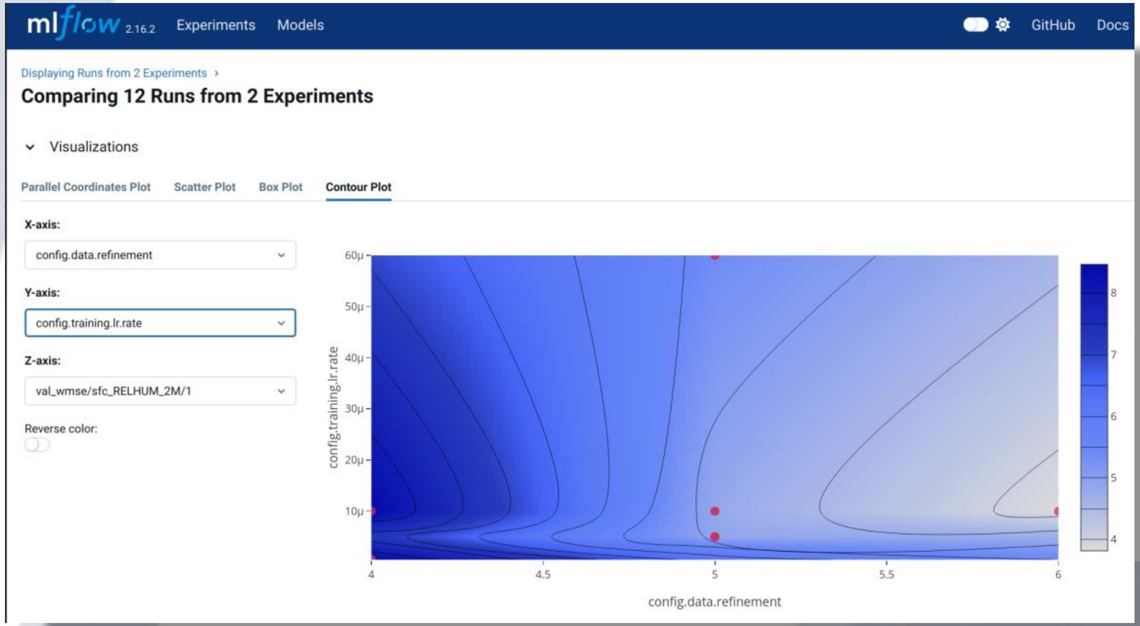




Mlflow web user interface

- Powerful tools to evaluate hyperparameters scans
- Box plots for single parameter dependency
- Contour plot for double parameter dependency





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Mlflow in the MLOps pipeline (current early setup, DWD example)

GitLab

mlflow

mlflow

Code base

Experiments
- Experiment tracking
- Metrics
- Metadata
- Models

Model registry
- Staging
- Promote experiments to models
- Versioning

Verification

Operations

Developer

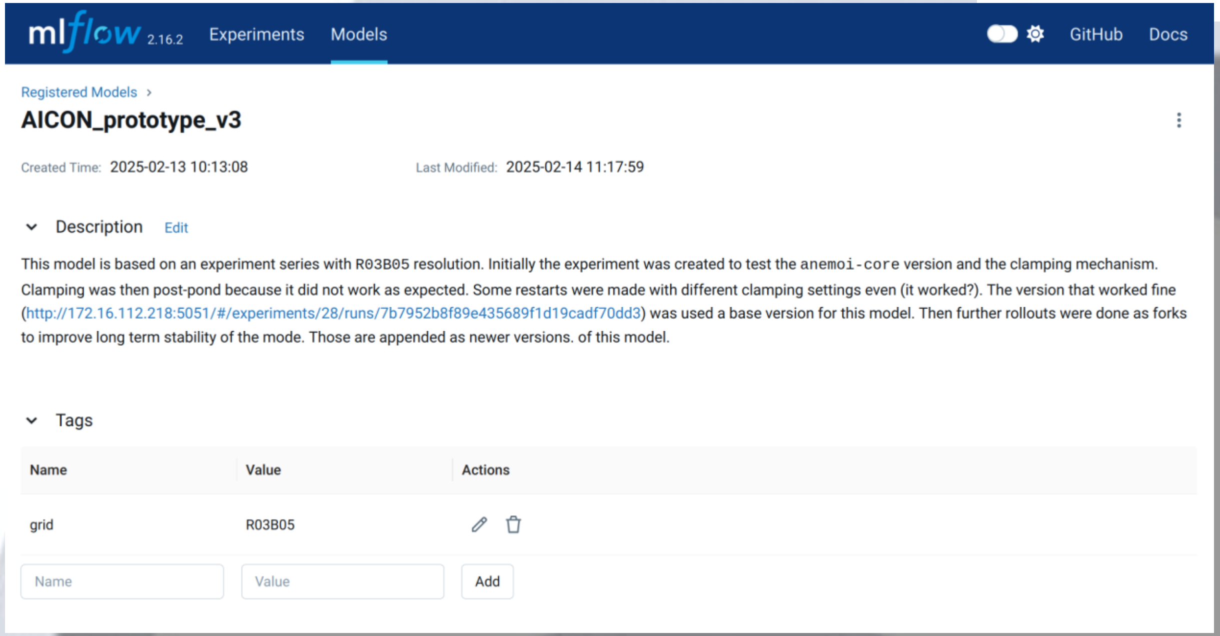
Researcher

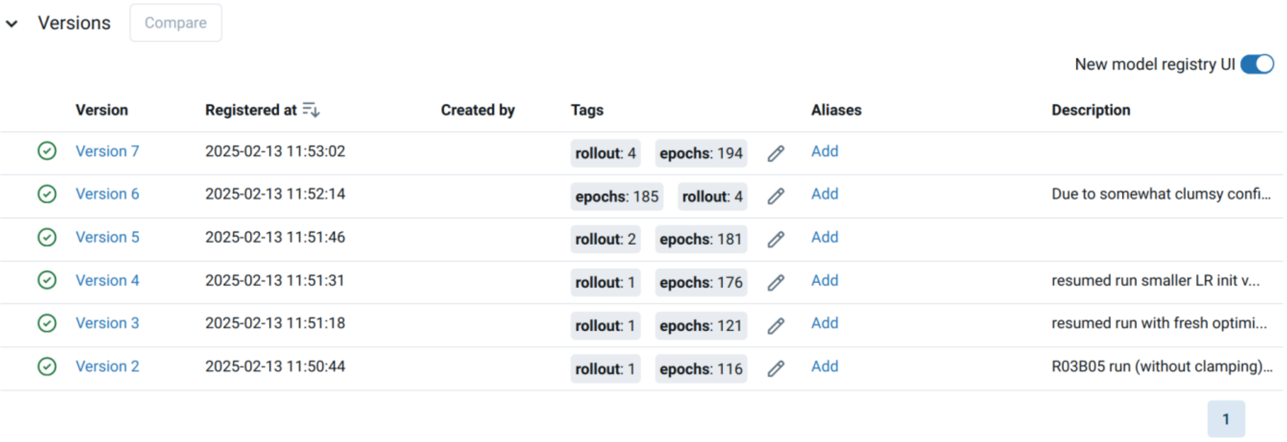
Operator

potentially new experiments?

Mlflow model registry

- Inference checkpoints can be logged as experiment artifacts
- These can be promoted to the model registry
- A model can have a description and tags
- Versions of that model can hold their own tags and descriptions
- Each version also links to a specific experiment run where the inference checkpoint can be found.
- The most interesting models can thus be stored in prominent place, augmented with information, potentially ready for inference
- @DWD we currently experiment with this tool. Use verisons to document training history.





Summary

- Organize experiments
- Reproducibility
- Evaluate hyperparameter studies
- Register models
- Transition to inference, routine verification and operations

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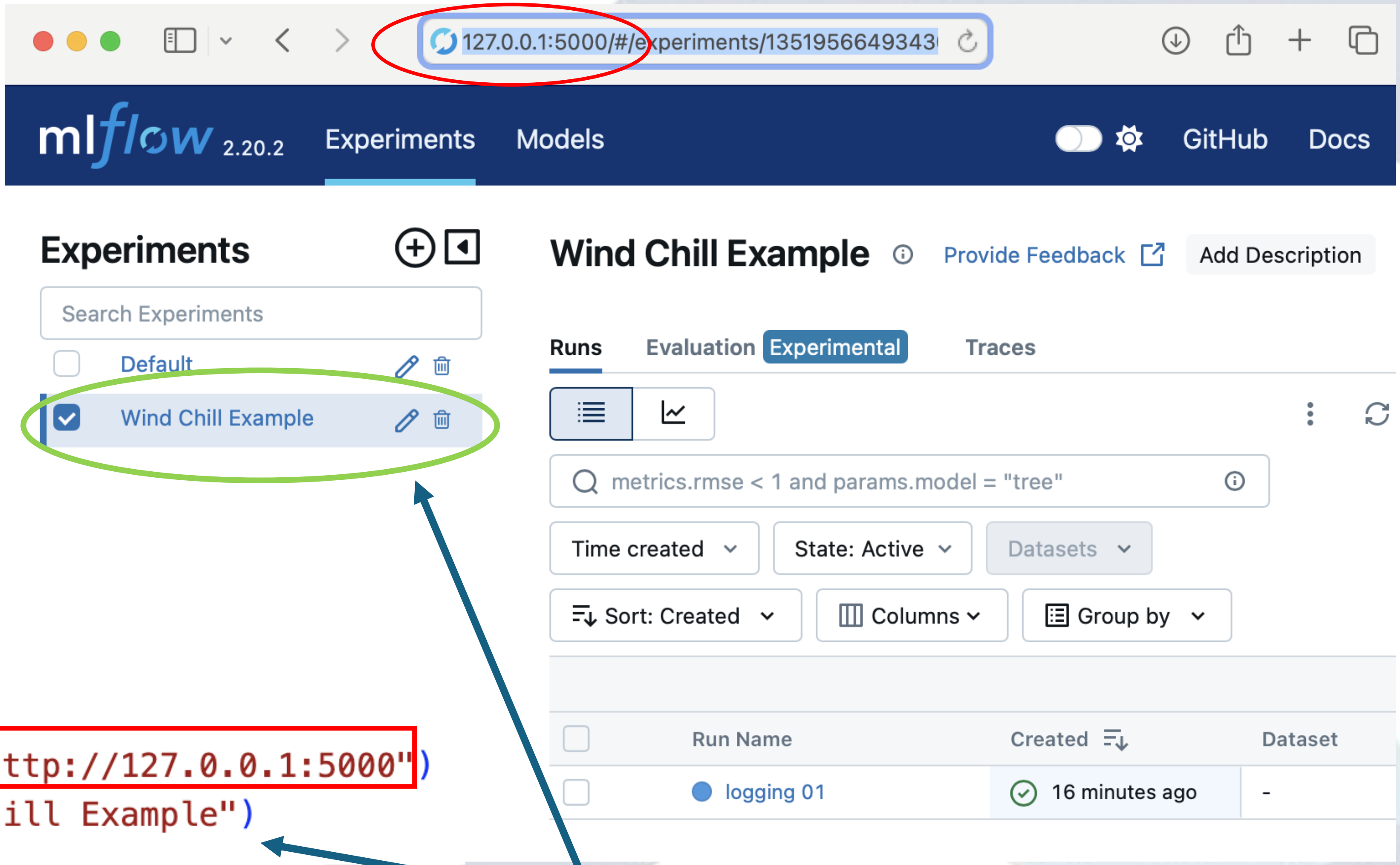
Logging in MLFlow

Step 1

Mlflow server for local experimentation

$ mlflow ui



Step 2

```python
#Set up MLflow
import mlflow
mlflow.set_tracking_uri(uri="http://127.0.0.1:5000")
mlflow.set_experiment("Wind Chill Example")
```

Experiment name

Logging in MLFlow

Start an MLflow run

Log parameters

Set tag

Training loop

Log metrics

```
with mlflow.start_run(run_name="logging 01"):

  # Log the hyperparameters
    mlflow.log_params({ "hidden_dim": hidden_dim})

    mlflow.set_tag("Training Info", "Basic model for wind chill prediction")

    for epoch in range(n_epoch):
        optimizer.zero_grad()  # Clear gradients

        y_pred = model(x_train)  # Forward pass

        loss = criterion(y_pred, y_train)  # Compute loss
        loss.backward()  # Backpropagate error
        optimizer.step()  # Update weights

        train_loss.append(loss.item())  # Save loss

        y_pred=model(x_val) # predict on validateion dataset
        vloss=criterion(y_pred,y_val)

        # Log the losses metrics
        mlflow.log_metric("loss", loss.item(), step=(epoch+1))
        mlflow.log_metric("val_loss", vloss.item(), step=(epoch+1))
```

Logging in MLFlow

Model signature

```
# Infer the model signature
signature = infer_signature(x_train, model(x_train))
```

Log model

```
# Log the model
mlflow.pytorch.log_model(model, "model", signature=signature)
```

Log figure

```
# Log the figure
mlflow.log_figure(plt.gcf(), "figure.png")
```

Link

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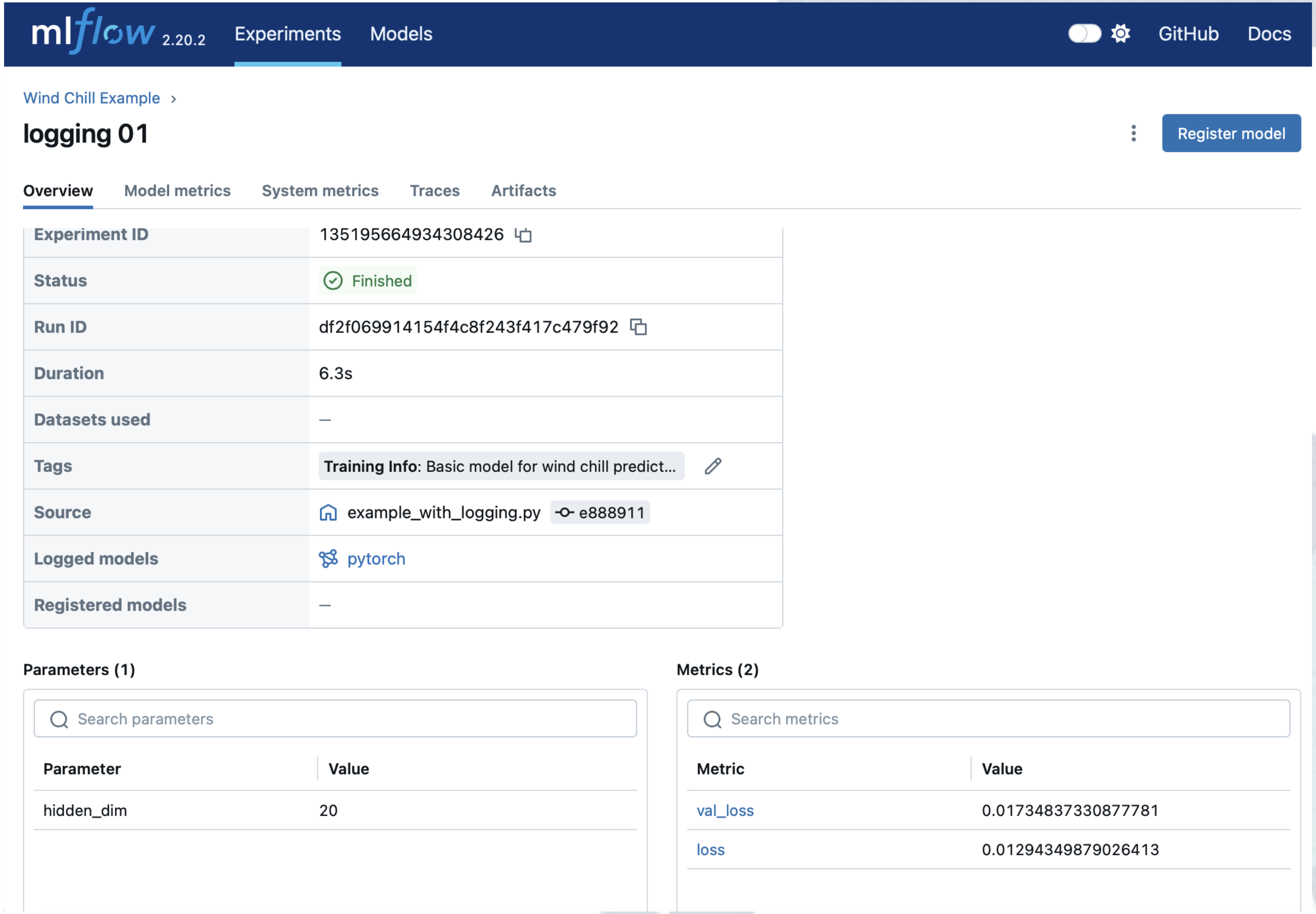
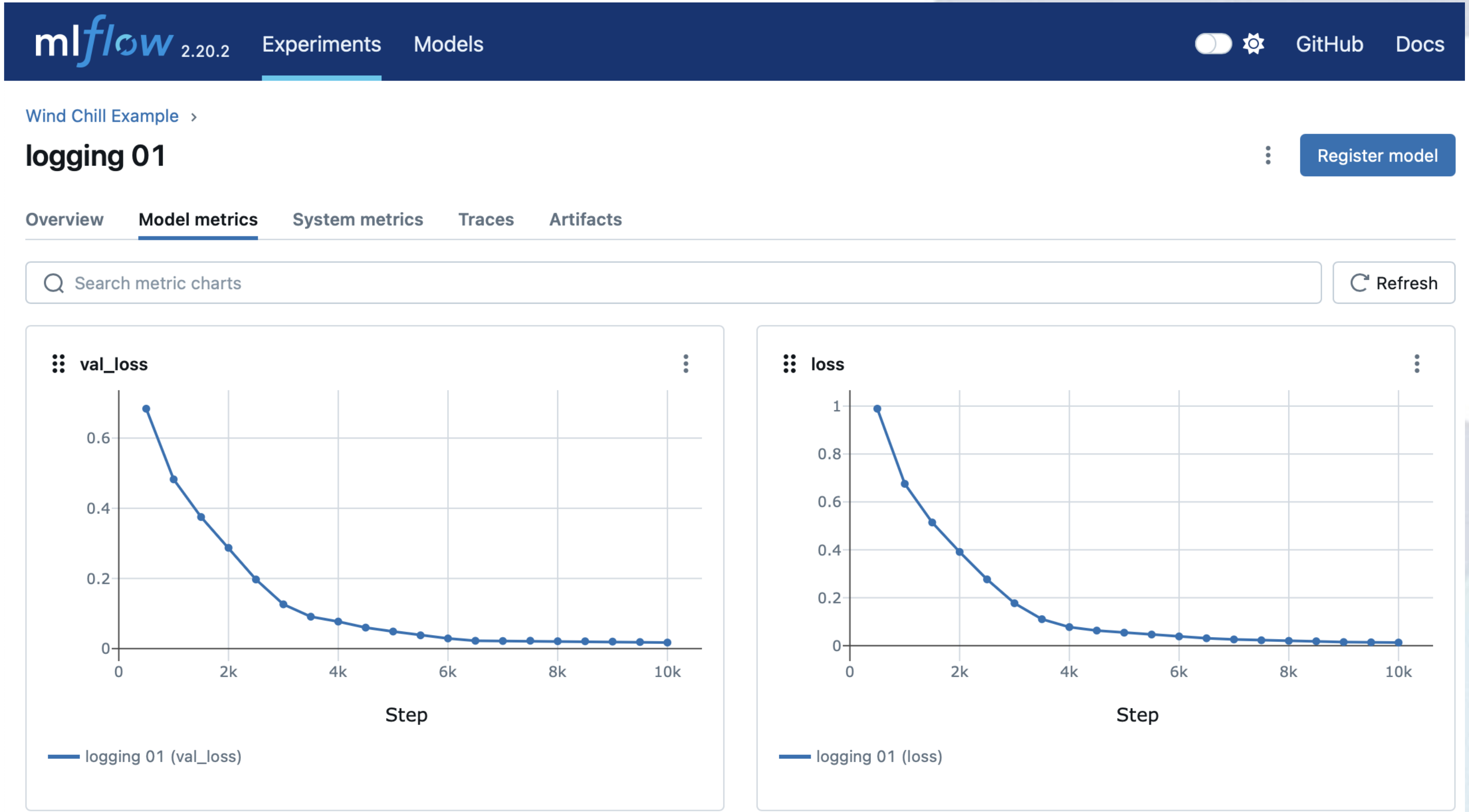
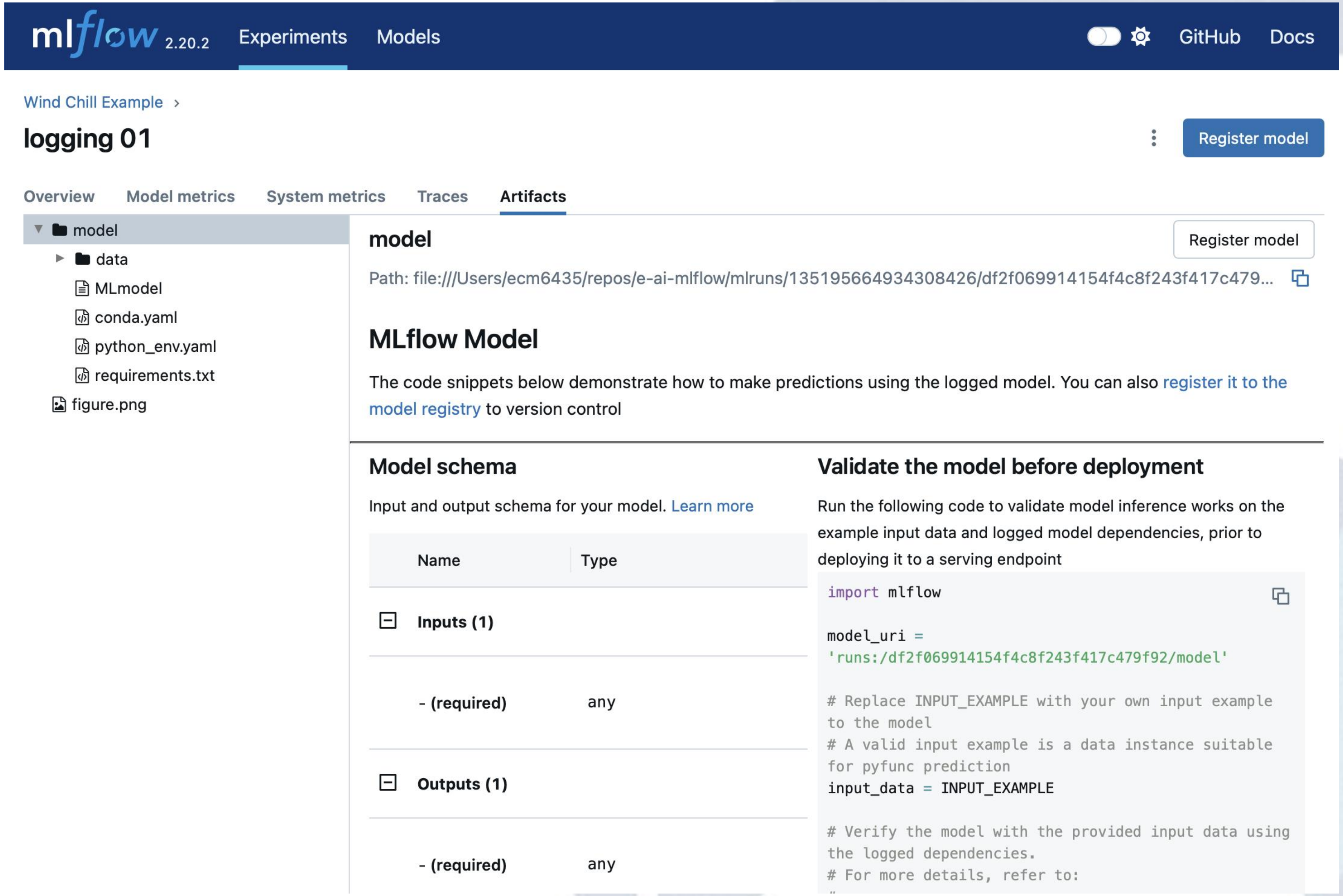
Logged Run in UI



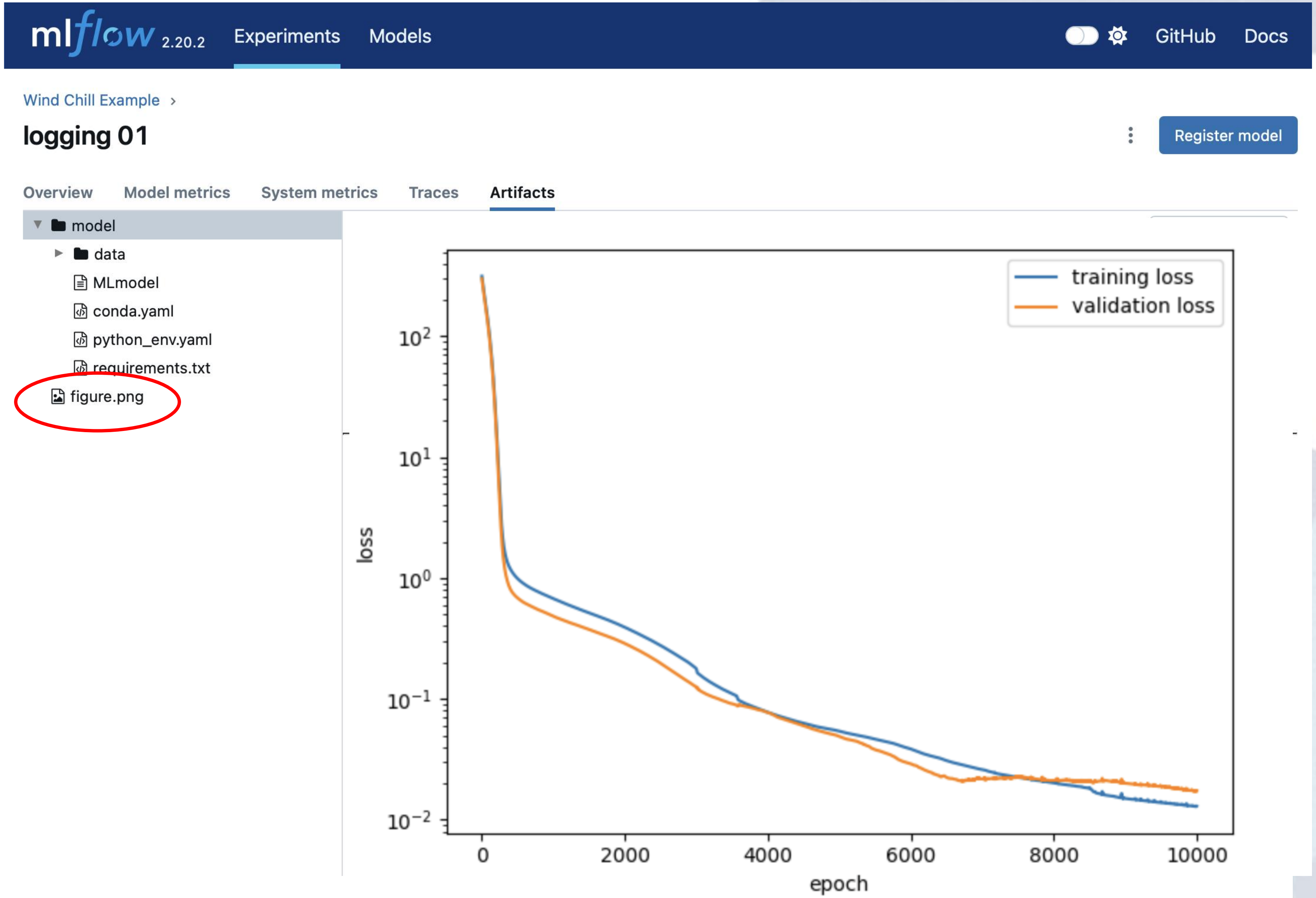
Logged Run in UI



Logged Run in UI



Logged Run in UI



Logging to the ECMWF MLflow server

Before starting a training run, you need to authenticate yourself to the MLflow server and obtain a token. <u>A valid token is required before starting training.</u>

This is done with the `anemoi-training mlflow login` command.

The first time you run the command, you need to pass the URL with `--url` and you need to obtain a seed token:

```
$ anemoi-training mlflow login --url https://mlflow.ecmwf.int

2024-10-14 10:54:10 INFO 🌐 Logging in to https://mlflow.ecmwf.int
2024-10-14 10:54:10 INFO 📝 Please obtain a seed refresh token from https://mlflow.ecmwf.int/seed
2024-10-14 10:54:10 INFO 📝 and paste it here (you will not see the output, just press enter after pasting):
Refresh Token: ***
2024-10-14 11:00:17 INFO Your MLflow login token is valid until 2024-11-12 11:00:17 UTC
2024-10-14 11:00:17 INFO ✅ Successfully logged in to MLflow. Happy logging!
```

Logging to the ECMWF MLflow server using the AnemoiMLflowClient

Unless your codebase is compatible with anemoi-training, it's recommended to install it without dependencies:

```
$ pip install anemoi-utils mlflow
$ pip install anemoi-training --no-deps
```

pip might complain about missing dependencies, but you can ignore that.

You can use the custom mlflow client with authentication like this. It behaves like a normal `mlflow.MlflowClient` :

```
from anemoi.training.diagnostics.mlflow.client import AnemoiMlflowClient

client = AnemoiMlflowClient("https://mlflow.ecmwf.int", authentication=True)

# do regular mlflow client things
client.search_experiments()
client.log_artifact(...)
```

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5.3 Running MLflow server as a user

and as a multi-user service

Run MLflow offline

```
import mlflow
with mlflow.start_run():
    mlflow.log_param("lr", 0.001)
```

If **tracking_uri is not specified**, MLflow logs data into local **mlruns directory**.

```
$ cat mlruns/0/7d*/params/lr
0.001
```

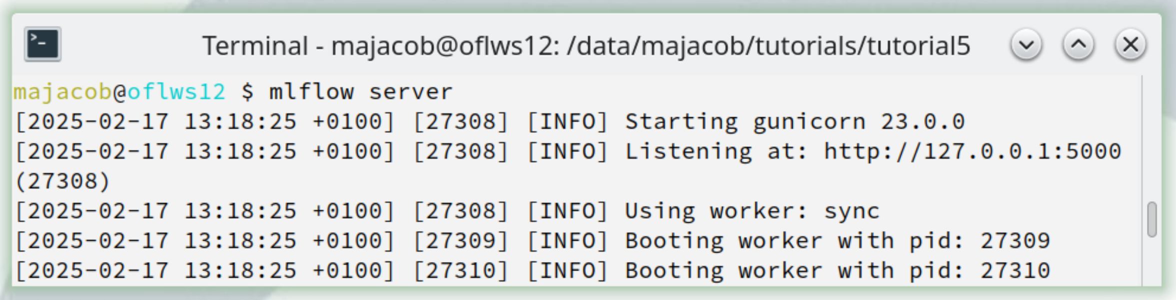
```
majacob@oflws12 $ tree
.
└── mlruns/
    ├── 0/
    │   ├── 7d0eebb3d24c485c9bc318c395d14449/
    │   │   ├── artifacts/
    │   │   ├── meta.yaml
    │   │   ├── metrics/
    │   │   ├── params/
    │   │   │   └── lr
    │   │   └── tags/
    │   │       ├── mlflow.runName
    │   │       ├── mlflow.source.name
    │   │       ├── mlflow.source.type
    │   │       └── mlflow.user
    │   └── meta.yaml
    └── models/

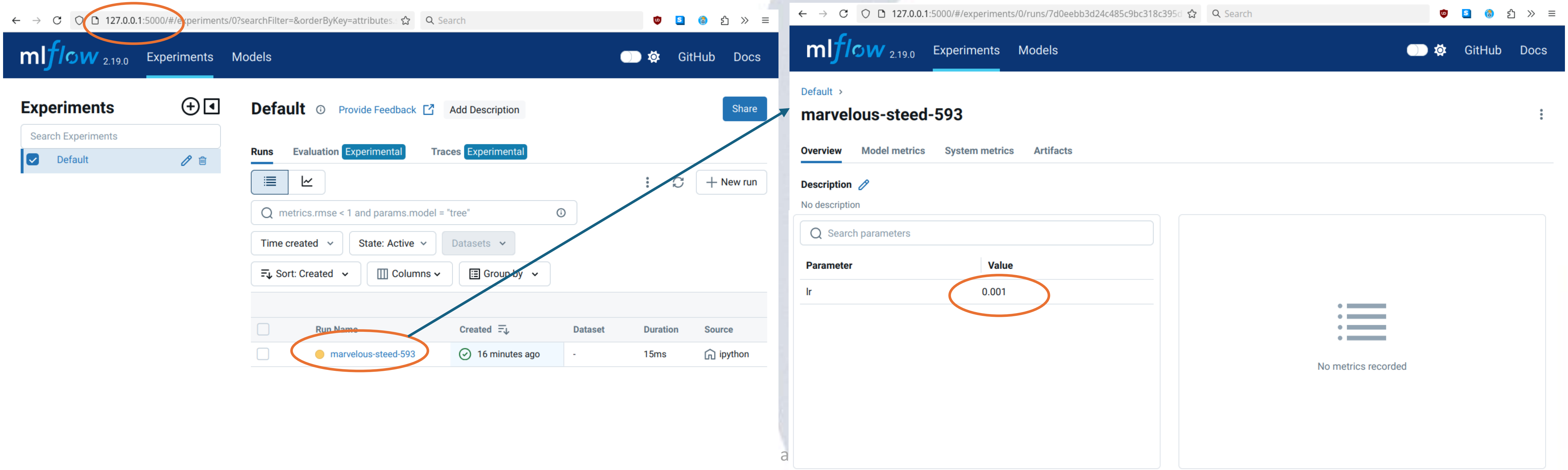
8 directories, 7 files
```

Visualization with MLflow

```
$ mlflow server
# or
$ mlflow ui # alias for server
```

"Server" is available at http://127.0.0.1:5000
(for all users of localhost)



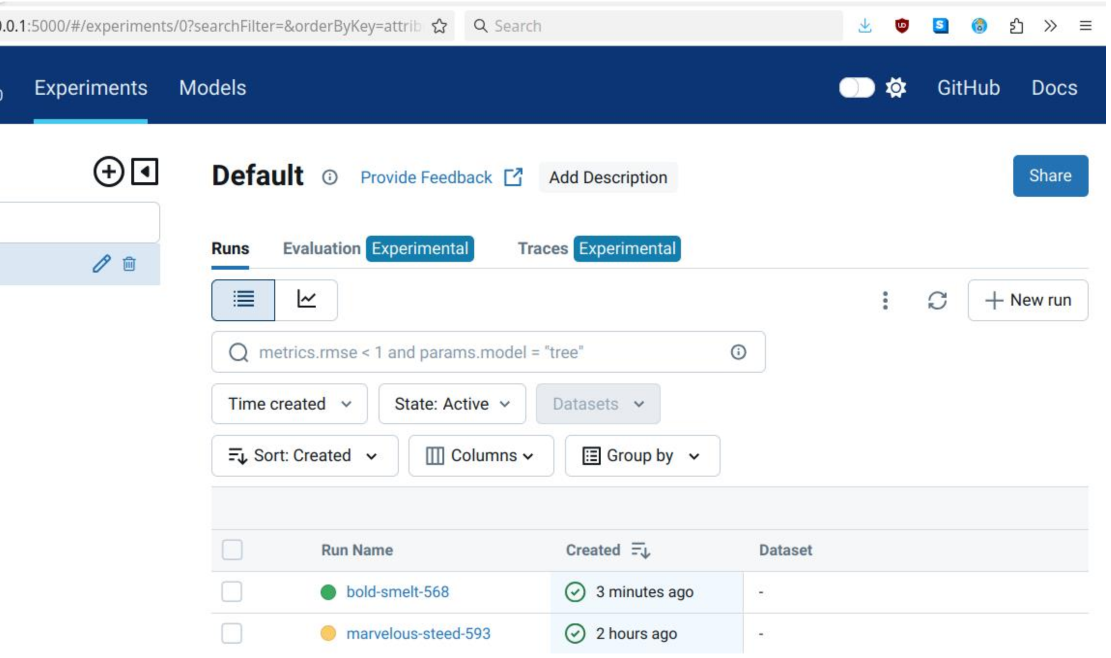


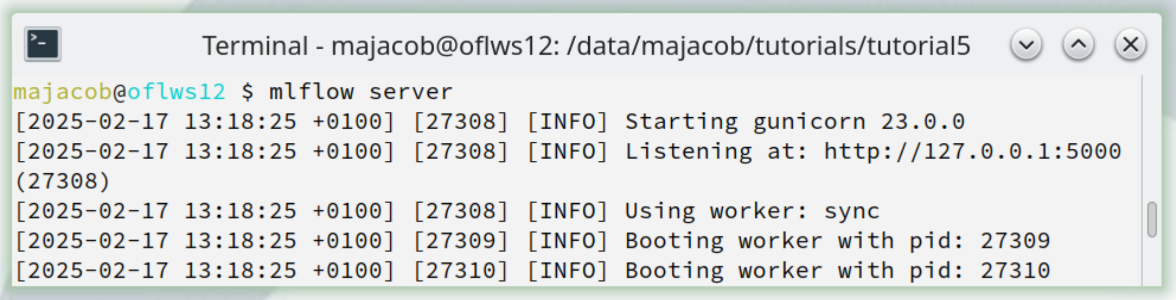
MLflow tracking server

- MLflow tracking server is a stand-alone HTTP server that serves multiple REST API endpoints for tracking runs/experiments
- **Collaboration**: Multiple users can log runs to the same endpoint, and query runs and models logged by other users.
- **Sharing Results**: The tracking server also serves Tracking UI endpoint, where team members can easily explore each other's results.
- **Centralized Access**: The tracking server can be run as a proxy for the remote access for metadata and artifacts, making it easier to secure and audit access to data.

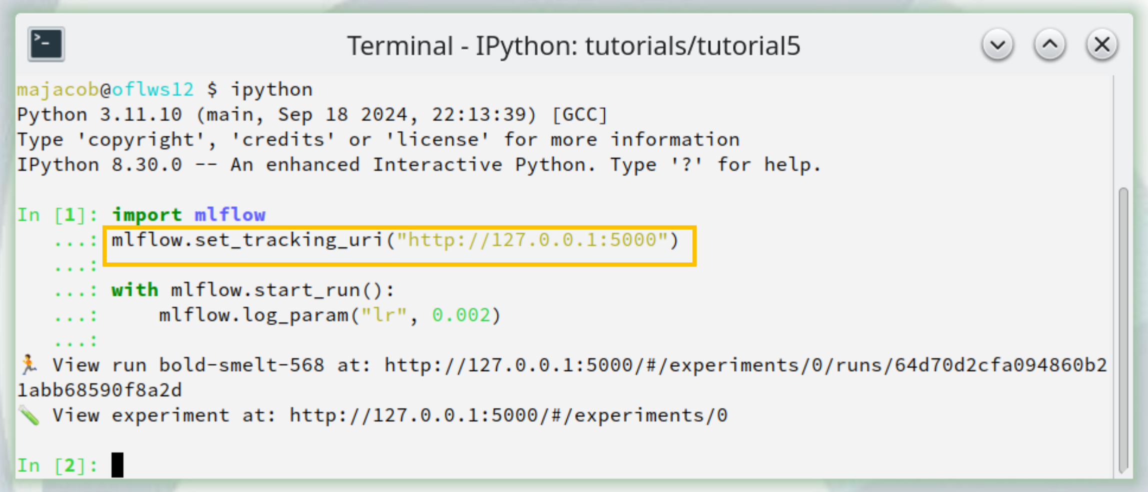
https://mlflow.org/docs/latest/tracking/tutorials/remote-server.html

MLflow server





Communication via network
Internal REST API



127.0.0.1:5000 is available to all users on the host!

From local server to network server

- Open server to other hosts in the network

```
mlflow server --host 0.0.0.0 --port 5000
```

(port is optionally)

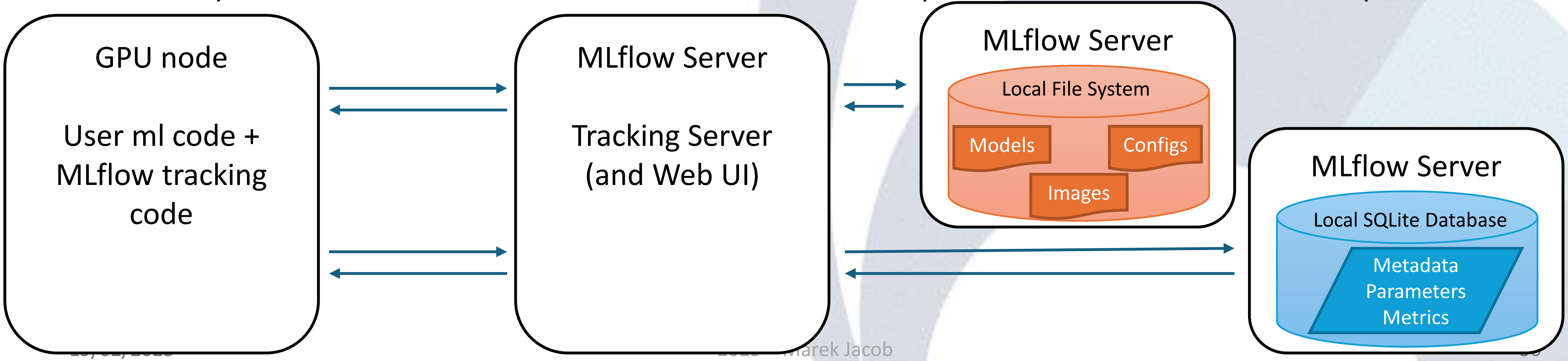
-- host: The network address to listen on (default: 127.0.0.1).
Use 0.0.0.0 to bind to all addresses if you want to access the tracking server from other machines.

Assumption: Your machine is part of a trusted network.

Advice: implement **authentication** and **encryption** if the server is connected directly to the internet.

Storage backends

- **Backend store**: Database to store all metadata, parameters and metrics.
  Default: file based (limited performance, many small files).
  Improved performance with SQLAlchemy-compatible **database** (e.g., SQLite, PostgreSQL, MySQL).
  `--backend-store-uri "sqlite:///${DIR}/mlflow-store.db“`
- **Artifact store**: Store images, models, configs, etc.
  E.g. Amazon S3 and S3-compatible storage; Azure Blob Storage; Google Cloud Storage; (S)FTP server; NFS; HDFS; local file system
  `--artifacts-destination "${DIR}/mlflow-artifacts“`
  MLflow server proxies access to artifacts
  - Only MLflow server sees bucket credentials and uses the permissions of the mlflow server process



Basic Authentication

- `export MLFLOW_AUTH_CONFIG_PATH="${DIR}/auth_config.ini“`
  `mlflow server --app-name basic-auth`
- Implements basic HTTP authentication with **username** and **password**

auth_config.ini

```
[mlflow]
default_permission = READ
database_uri = sqlite:////work/some/path/basic_auth.db
admin_username = admin
admin_password = to-be-changed
authorization_function = mlflow.server.auth:authenticate_request_basic_auth
```

Update the default admin password as soon as possible!

- “This feature is still experimental and may change in a future release without warning.”
- (“admin” user is mandatory)

https://mlflow.org/docs/latest/auth/index.html

Basic Authentication

- ```
  export MLFLOW_AUTH_CONFIG_PATH="${DIR}/auth_config.ini“
  mlflow server --app-name basic-auth
  ```
- Implements basic HTTP authentication with **username** and **password**

```
auth_config.ini
[mlflow]
default_permission = READ
database_uri = sqlite:////work/some/path/basic_auth.db
admin_username
admin_password
authorization_f                                          sic_auth
```

as soon as possible!

```
sqlite:////work/some/path/basic_auth.db
```
Protocol: `sqlite://`
Host: *(empty)*
Separator between Host and Path: `/`
Path (absolute or relative): `/work/some/path/basic_auth.db`
→ https://docs.sqlalchemy.org/en/13/dialects/sqlite.html#connect-strings

- “This feat   ease without w
- (“admin” user is mandatory)

https://mlflow.org/docs/latest/auth/index.html
```

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User Administration via Python API

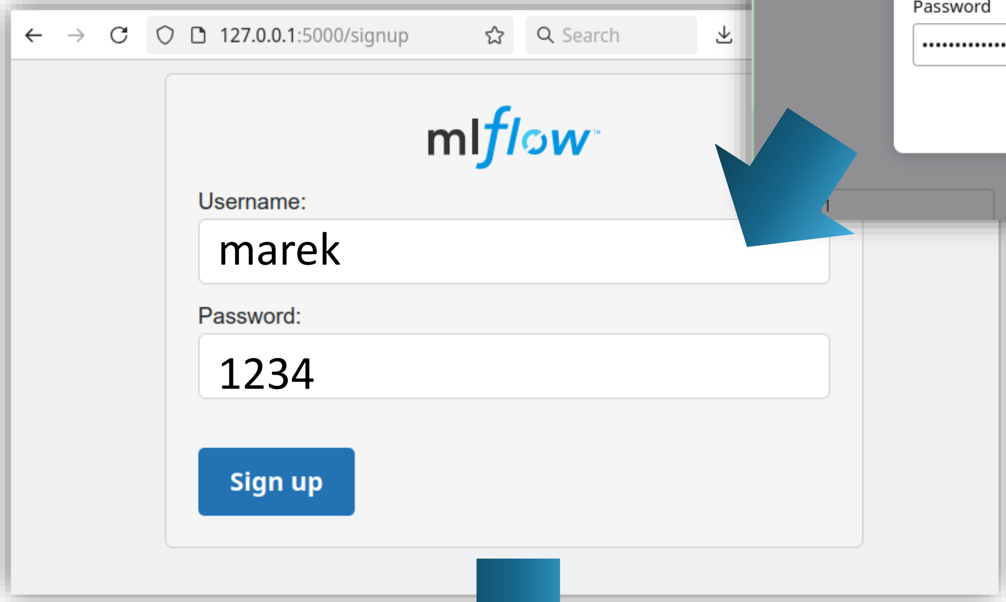
```
$ MLFLOW_TRACKING_USERNAME=admin MLFLOW_TRACKING_PASSWORD=to-be-changed ipython
IPython 8.30.0 -- An enhanced Interactive Python. Type '?' for help.

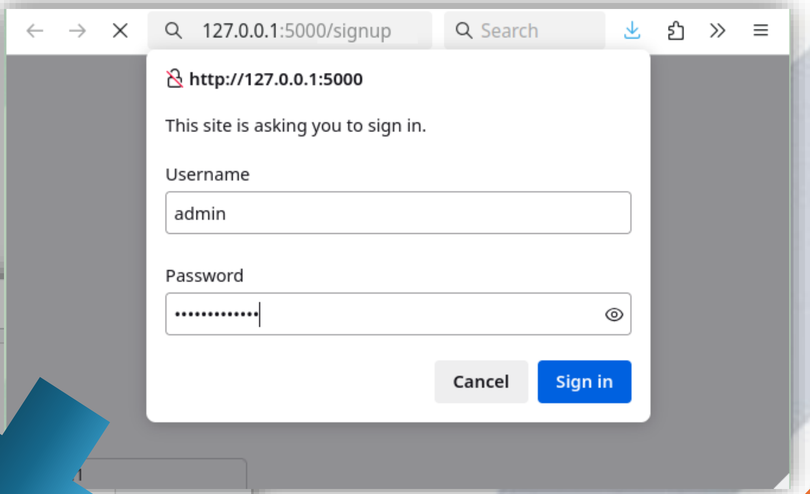
In [1]: from mlflow.server import get_app_client
from getpass import getpass
tracking_uri = "http://127.0.0.1:5000/"
user = "admin"
# do not `password = "my_new_password"`! Ipython would log the new password
password = getpass(f"Please enter a new password:\n“)
auth_client = get_app_client("basic-auth", tracking_uri=tracking_uri)
auth_client.update_user_password(user, password)
```

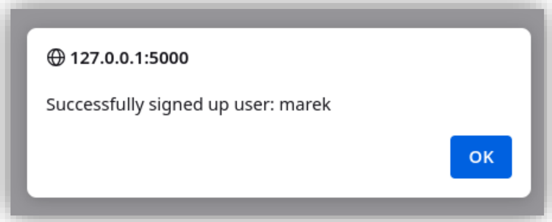
Further API endpoints for permissions, user creation, etc. available in the documentation:
https://mlflow.org/docs/latest/auth/index.html

Add New User

127.0.0.1:5000/signup







Provide Credentials to MLflow Client

```
$ mkdir ~/.mlflow
$ touch ~/.mlflow/credentials
$ chmod 600 ~/.mlflow/credentials
$ vim ~/.mlflow/credentials
```

```
~/.mlflow/credentials
[mlflow]
mlflow_tracking_username = marek
mlflow_tracking_password = 1234
```

Alternative Environment Variables:
MLFLOW_TRACKING_USERNAME
MLFLOW_TRACKING_PASSWORD

User Setup Convenience

```
majacob@oflws12 $ python mlflow_setup.py
/home/majacob/.mlflow/credentials does not exist...
    ... create a new one
Please enter your mlflow username for server http://localhost:5000/:
marek
Please enter your mlflow (initial) password:
   ← Enter 1234 secretly
    ... testing user marek
    ... testing user marek
Please enter a new password for mlflow on http://localhost:5000/:

Please repeat that password:

    ... password updated in /home/majacob/.mlflow/credentials
    ... an successfully tested on http://localhost:5000/
```

```
majacob@oflws12 $ cat ~/.mlflow/credentials
[mlflow]
mlflow_tracking_username = marek
mlflow_tracking_password = 1234
```

mlflow_setup.py

```python
import configparser
from getpass import getpass
import os
import sys
import pathlib

from mlflow.server import get_app_client

# Configure you ml flow server
tracking_uri = "http://localhost:5000/"


def setup_config(config_file):
    """
    """
    print(f"{config_file} does not exist...")
    print("    ... create a new one")

    config_file.parent.mkdir(mode=0o700, parents=True, exist_ok=True)
    user = input(f"Please enter your mlflow username for server {tracking_uri}:\n")
    password = getpass(f"Please enter your mlflow (initial) password:\n")

    # create empty file
    open(config_file, "w").close()

    # set permissions to user read/write only
    config_file.chmod(0o600)

    with open(config_file, "a") as f:
        f.write("[mlflow]\n")
        f.write(f"mlflow_tracking_username = {user}\n")
        f.write(f"mlflow_tracking_password = {password}\n")

    try:
        print(f"    ... testing user {user}")
        test_connection(user)
    except Exception as e:
        print(e)
        print("Wrong username or password.")
        os.remove(config_file)
        print(f"    ... deleting {config_file}")
        sys.exit(1)


t_connection(user):
client = get_app_client("basic-auth", tracking_uri=tracking_uri)
```

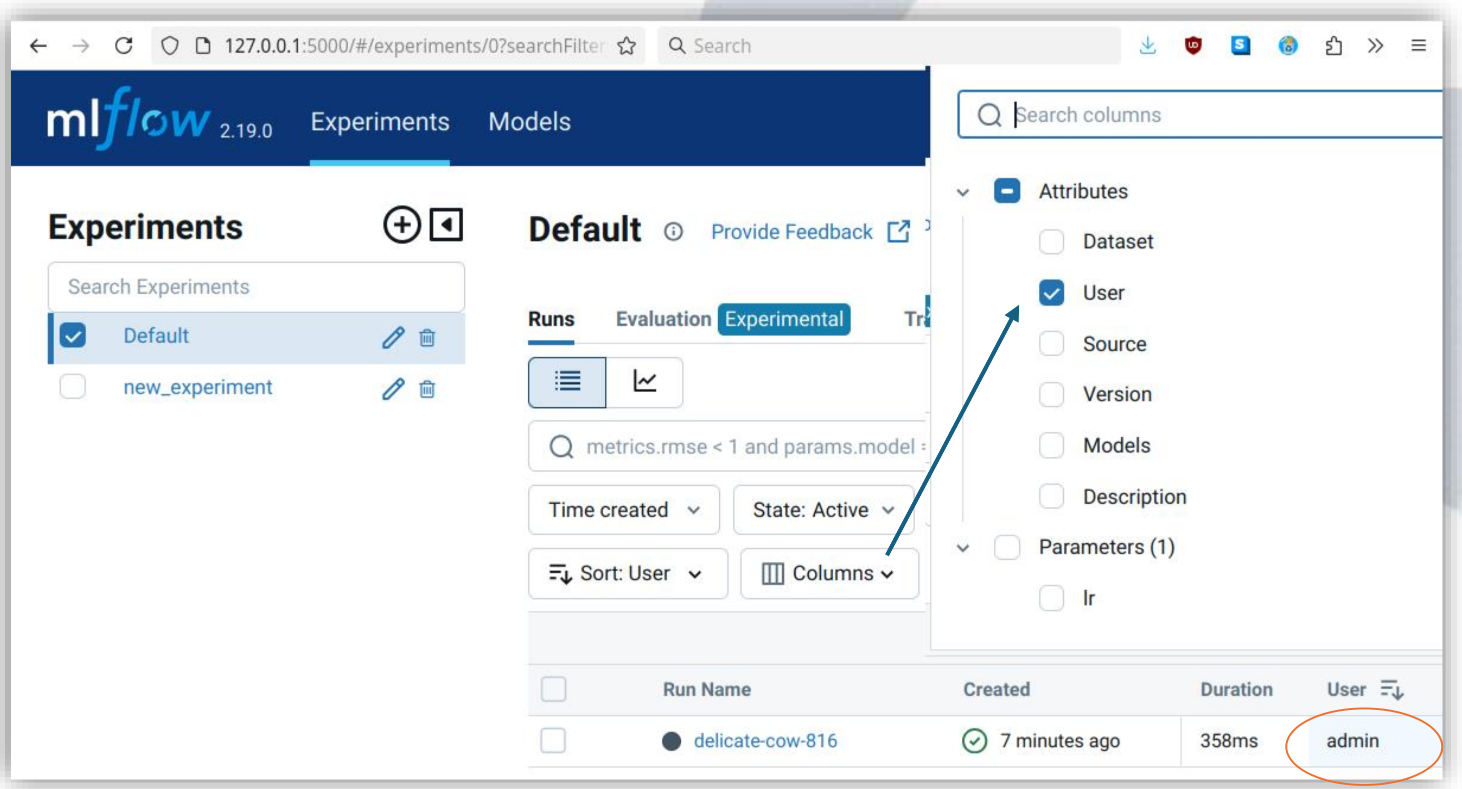
MLflow permissions

- User can not delete/edit foreign experiments
- User can not extend foreign experiments
  - Can't log to "Default" experiment
  - Start new experiment:

```
mlflow.set_experiment(“new_experiment")
```

```
In [1]: import mlflow
   ...: mlflow.set_tracking_uri("http://127.0.0.1:5000")
   ...:
   ...: with mlflow.start_run():
   ...:     mlflow.log_param("lr", 0.002)
   ...:
---------------------------------------------------------------------------
MlflowException                           Traceback (most recent call last)
```

```
MlflowException: API request to endpoint
/api/2.0/mlflow/runs/create failed with error code 403
!= 200. Response body: 'Permission denied'
```



Recap: MLflow Server command

- `pip install mlflow`
- ```
  export MLFLOW_AUTH_CONFIG_PATH="${DIR}/auth_config.ini"
  export OPENBLAS_NUM_THREADS=1 # reduce virt. mem footprint
  mlflow server \
    --app-name basic-auth \
    --backend-store-uri "sqlite:///${DIR}/mlflow.db" \
    --artifacts-destination "${DIR}/mlflow-artifacts" \
    --workers 10 \ # increase number of workers
    --host 0.0.0.0 --port 5000
  ```
- Create user account using the admin account: http://127.0.0.1:5000/signup
- Use MLflow client API to change passwords
- Advanced steps for public MLflow server:
  - Hide MLflow server behind HTTPS Reverse Proxy (NGINX or Apache httpd)
  - Align authentication with institutional identity management (auth mechanism is pluginable)
  ```

Run MLflow in a Screen session

```
#!/usr/bin/env bash
set -e
DIR=$( cd -- "$( dirname -- "${BASH_SOURCE[0]}" )" &> /dev/null && pwd )
cd "$DIR"

SCREEN_SESSION=mlflow
export MLFLOW_AUTH_CONFIG_PATH="${DIR}/auth_config.ini"

export OPENBLAS_NUM_THREADS=1

send_to_screen(){
  # Replace occurrences of $ with \$ to prevent variable substitution:
  string="${1//$/\\$}"
  screen -xr $SCREEN_SESSION -X stuff "$string\r"
}

# start a detached screen session
screen -dmS $SCREEN_SESSION

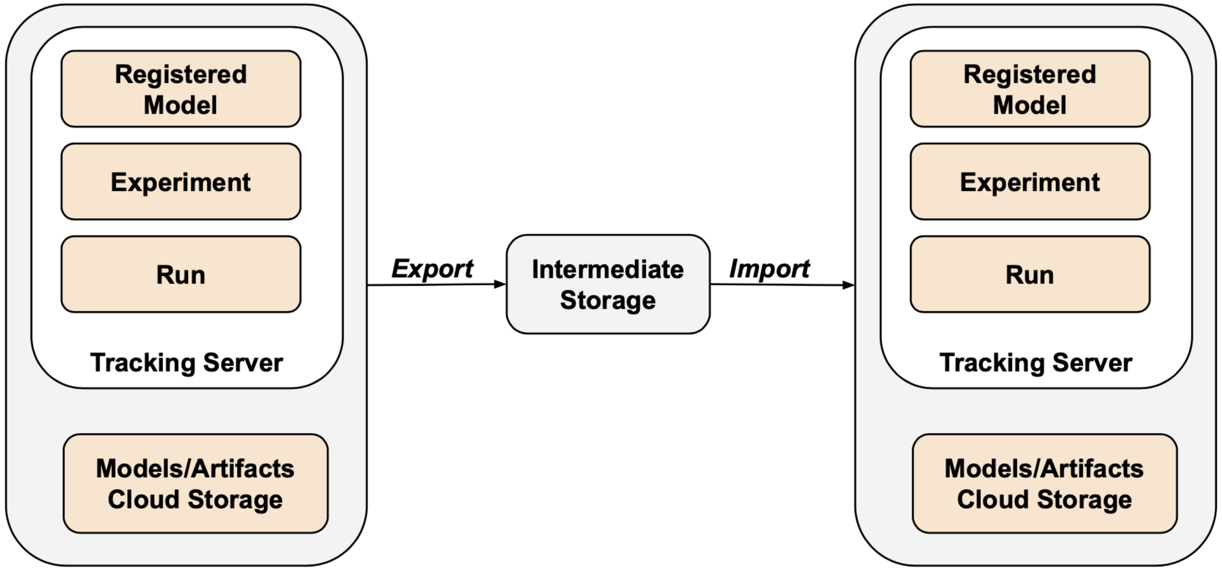
send_to_screen "date"
send_to_screen "echo \$PWD"
send_to_screen "echo \$MLFLOW_AUTH_CONFIG_PATH"
send_to_screen "source \"${DIR}/mlflow_venv/bin/activate\""
send_to_screen "mlflow server --app-name basic-auth --backend-store-uri \"sqlite:///${DIR}/mlflow.db\" --artifacts-destination
\"${DIR}/mlflow-artifacts\" --workers 10 --host 0.0.0.0 --port 5000"
echo "Started mlflow in a detached screen session."
echo "Enter \`screen -xr $SCREEN_SESSION\` to attach."
echo "Then press 'ctrl+a d' to detach."
```

GNU Screen

- Terminal multiplexer
- Virtual consoles (terminals) are organised in sessions
- Allows a user to detach and reattach a session
- Separates processes from login session
- (Alternative to tmux)

MLflow Export Import

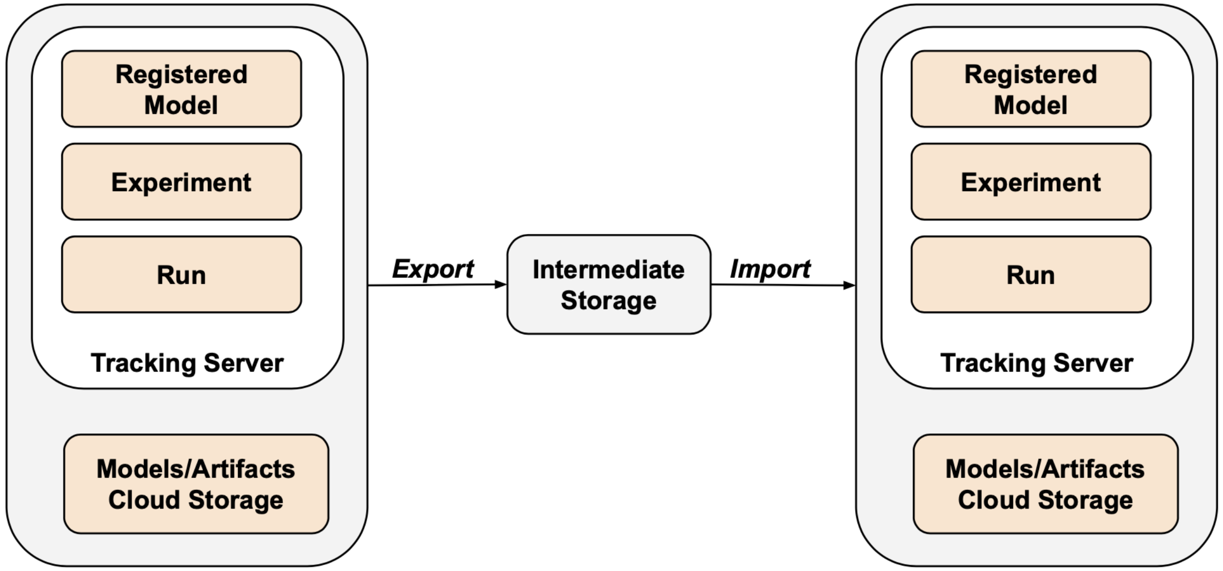
- Copy MLflow objects from one tracking server to another.
  - Also from file-based offline logging to a server.



- `pip install git+https:///github.com/mlflow/mlflow-export-import/#egg=mlflow-export-import`
- 1. Export:
```
export MLFLOW_TRACKING_URI=http://localhost:5000
# Note start `mlflow server` when exporting from file-based offline log
export-experiment --experiment Default --output-dir /tmp/export
```
- 2. Import:
```
export MLFLOW_TRACKING_URI=http://some.remote:5001
import-experiment --experiment-name Default2 --input-dir /tmp/export
```
- Authentication:
  only with environment variables or
```
export MLFLOW_TRACKING_URI=http://$USER:$PASS@some.remote:5001
```

MLflow Export Import

- Copy MLflow objects from one tracking server to another.
  - Also from file-based offline logging to a server.



- `pip install git+https:///github.com/mlflow/mlflow-export-import/#egg=mlflow-export-import`
- 1. Export:

```
export MLFLOW_TRACKING_URI=http://localhost:5000
# Note start `mlflow server` when exporting from f
export-experiment --experiment Default --output-di
```

- 2. Import:

```
export MLFLOW_TRACKING_URI=http://some.remote:5001
import-experiment --experiment-name Default2 --inp
```

- Authentication:
  only with environment variables or

```
export MLFLOW_TRACKING_URI=http://$USER:$PASS@some
```

Anemoi:
The `anemoi-training mlflow sync` command wraps mlflow-export-import.
https://anemoi.readthedocs.io/projects/training/en/latest/user-guide/tracking.html#logging-offline-and-syncing-with-an-online-server

Further features of MLflow

- Model Registry

```
from mlflow.models import infer_signature
signature = infer_signature(x_val.numpy(), model(x_val).detach().numpy())
model_info = mlflow.pytorch.log_model(model, "model", signature=signature)
```

- Deployment
  - MLflow can deploy a model and make its inference available via REST API

```
mlflow models serve -m runs:/<run_id>/model -p 5000
```

You can then send a test request to the server as follows:

```
curl http://127.0.0.1:5000/invocations -H "Content-Type:application/json"  --data '{"inputs": [[1, 2], [3, 4], [5, 6]]}'
```

  - Can also be generated as docker container
- MLflow Recipes (Pipelines)
  - Define Recipes by combining multiple Steps (individual ML operations, e.g. ingesting data, fitting an estimator, evaluating, deployment)
  - For smaller problems, that share typical building blocks
- Model Evaluation
  - MLflow offers default evaluation methods for LLMs and classical ML codes.

Summary - Running MLflow server as a user and as a multi-user service

- MLflow is a powerful multi-user monitoring tool
  - Collaboration
  - Sharing Results
  - Document Training Linage
- Supports distributed services
  - MLflow tracking server
  - Metadata, parameters and metrics server
  - Artifact server
- Access control
  - Simple HTTP auth
- Data migration between servers and offline runs possible
  - Mlflow-export-import (+ Anemoi-training wrapper)

Further Information on E-AI

- Slides available at GitHub

  https://github.com/eumetnet-e-ai/tutorials
- Recording will be available at EUMETNET SharePoint

  https://tlnt19059.sharepoint.com/:f:/r/sites/E-AI/Shared%20Documents/Tutorials
- Register for E-AI updates and SharePoint Access:

  marek.jacob@eumetnet.eu
- Contacts:
  - Tobias Göcke: Tobias.Goecke@dwd.de
  - Helen Theissen: Helen.Theissen@ecmwf.int
  - Marek Jacob: Marek.Jacob@dwd.de
- E-AI Working Group „WG3 Operations“ for exchange on MLOps

  https://chat.europeanweather.cloud

E-AI Basic Tutorials

Tutorial E-AI Basics 4: January Wednesday 22, 2025, 11-12 CET
"MLOps" - Machine Learning Operations
4.1 Overview (20') [RP]
4.2 MLOps in relation to traditional Weather forecasting (20') [MJ]
4.3 Road to MLOps (20’) [DN]

Tutorial E-AI Basics 5: February Wednesday 19, 2025, 11-12 CET
MLflow - an open-source platform for managing the machine learning lifecycle
5.1 Overview - User perspective (20') [TG]
5.2 Logging to MLflow as a ML software developer (20') [HT]
5.3 Running MLflow server as a user and as a service (20') [MJ]

Tutorial E-AI Basics 6: **February Wednesday 26**, 2025, 11-12 CET
CI/CD - Continuous Integration and Continuous Deployment of ML codes
6.1 Overview – What can CI/CD do for you? (20') [MJ]
6.2 Basic tests with Pytest (20') [JD]
6.3 Setting up a runner (20') [FP]

AI generated Image,
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