CERN
openlab

AI workflow lifecycle on Digital Twins for multi-sciences

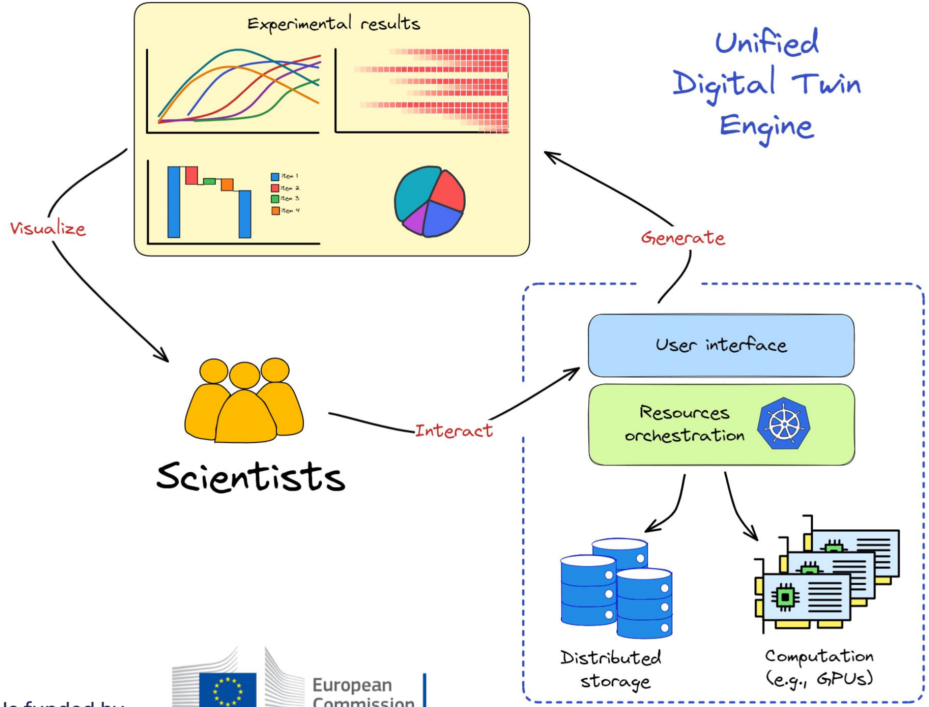
Matteo Bunino (matteo.bunino@cern.ch), Alexander Zoechbauer, Kalliopi Tsolaki, Rakesh Sarma, Ilaira Luise, Maria Girone, Sofia Vallecorsa

interTwin - Digital Twin Engine for science

Co-design and implement the prototype of an **interdisciplinary Digital Twin Engine**

Open-source platform based on **open standards**

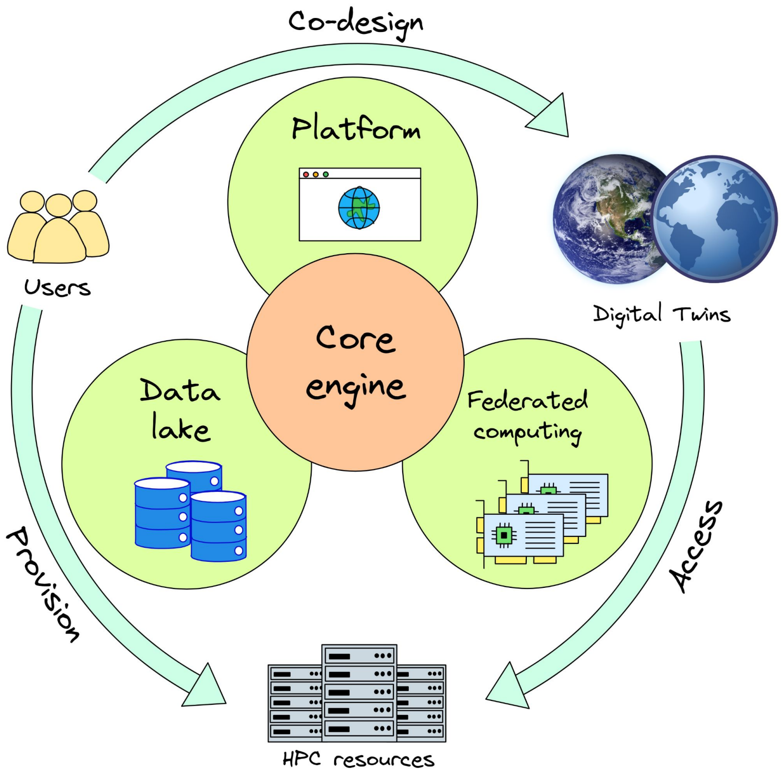
Large spectrum of **diverse use cases** from **physics** and **earth observation** sciences



Website: https://www.intertwin.eu/

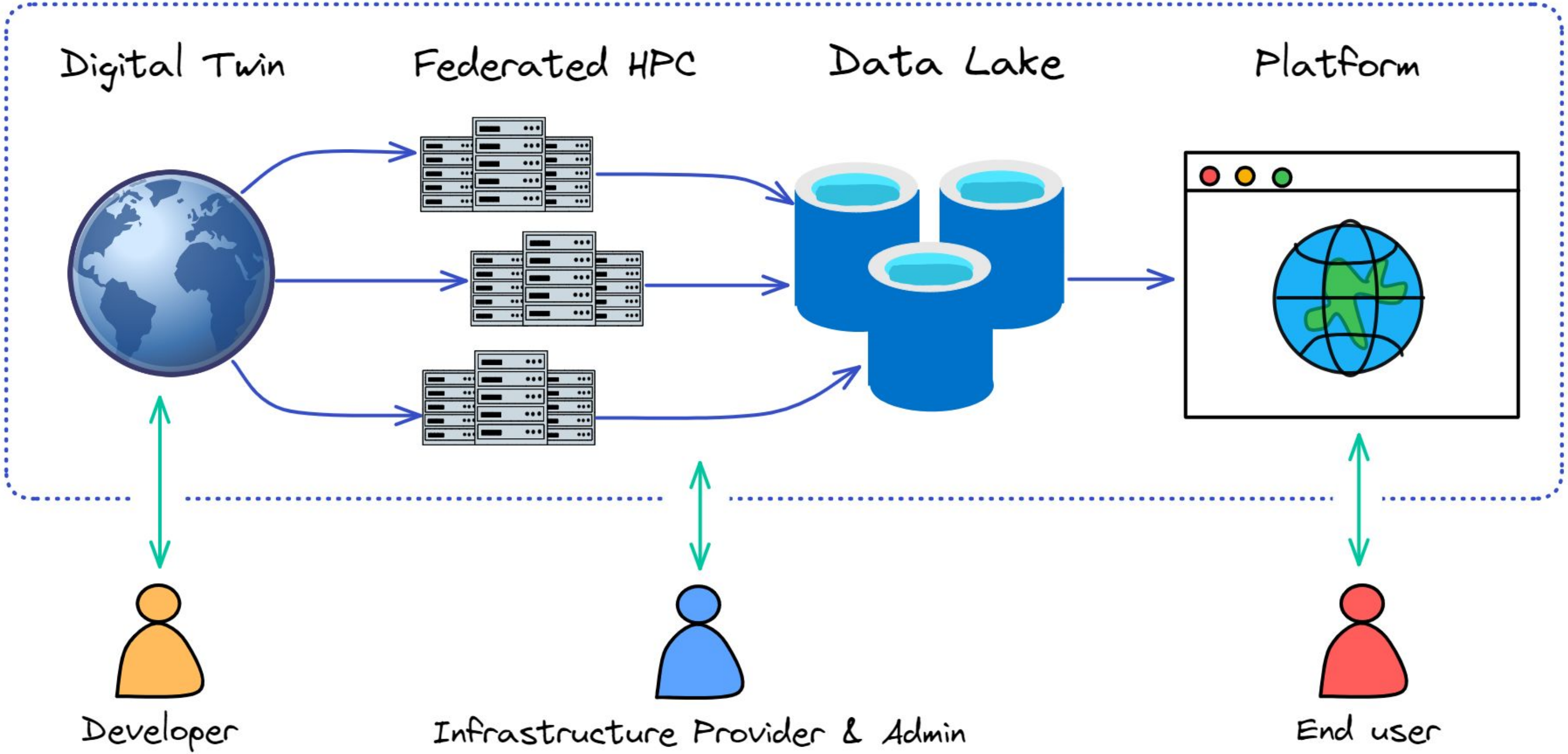
interTwin Is funded by European Commission

interTwin - Digital Twin Engine for science



interTwin

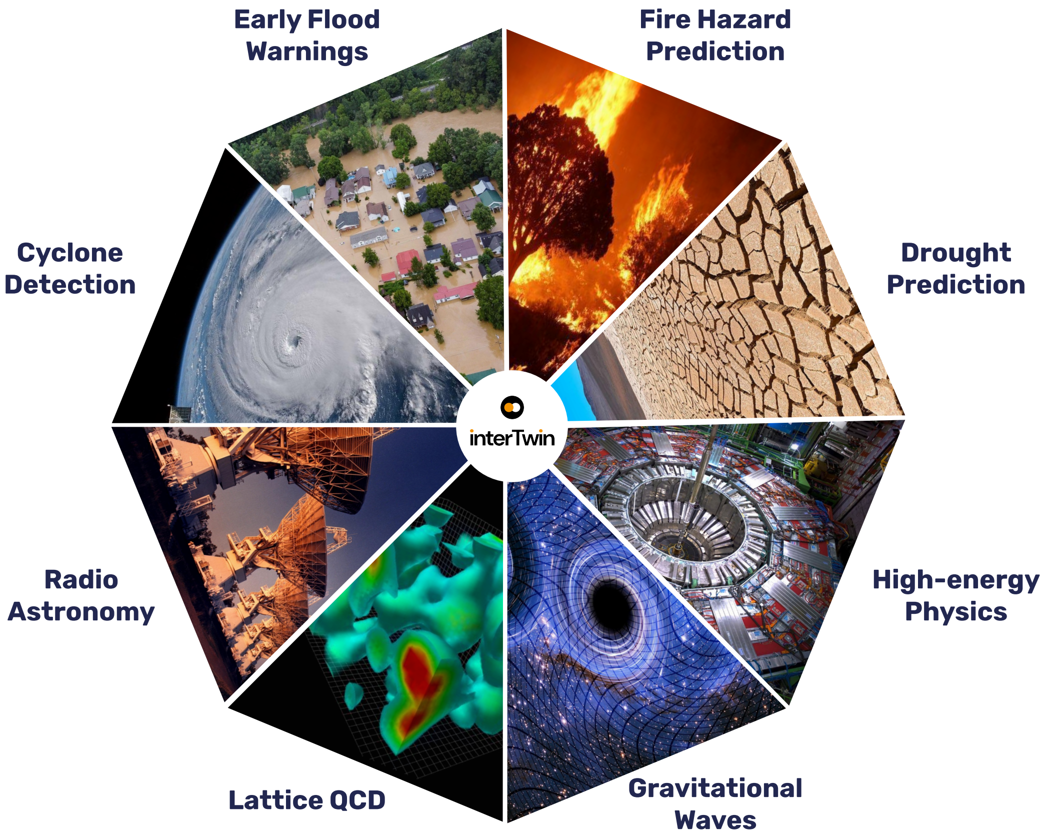
interTwin - Digital Twin Engine for science



interTwin

Multi-sciences DTs

interTwin use cases



interTwin

Earth Observation Use Cases in InterTwin

Cyclone Detection
CMCC, CNRS, Univ. of Torino

Fire Hazard Map Generation
CMCC, CNRS, Univ. of Torino

Early Flood Warnings
Deltares, EURAC, Technical Univ. of Vienna

Drought Prediction
CERFACS, EURAC, Deltares

interTwin

Climate Change Future Projections of Extreme Events

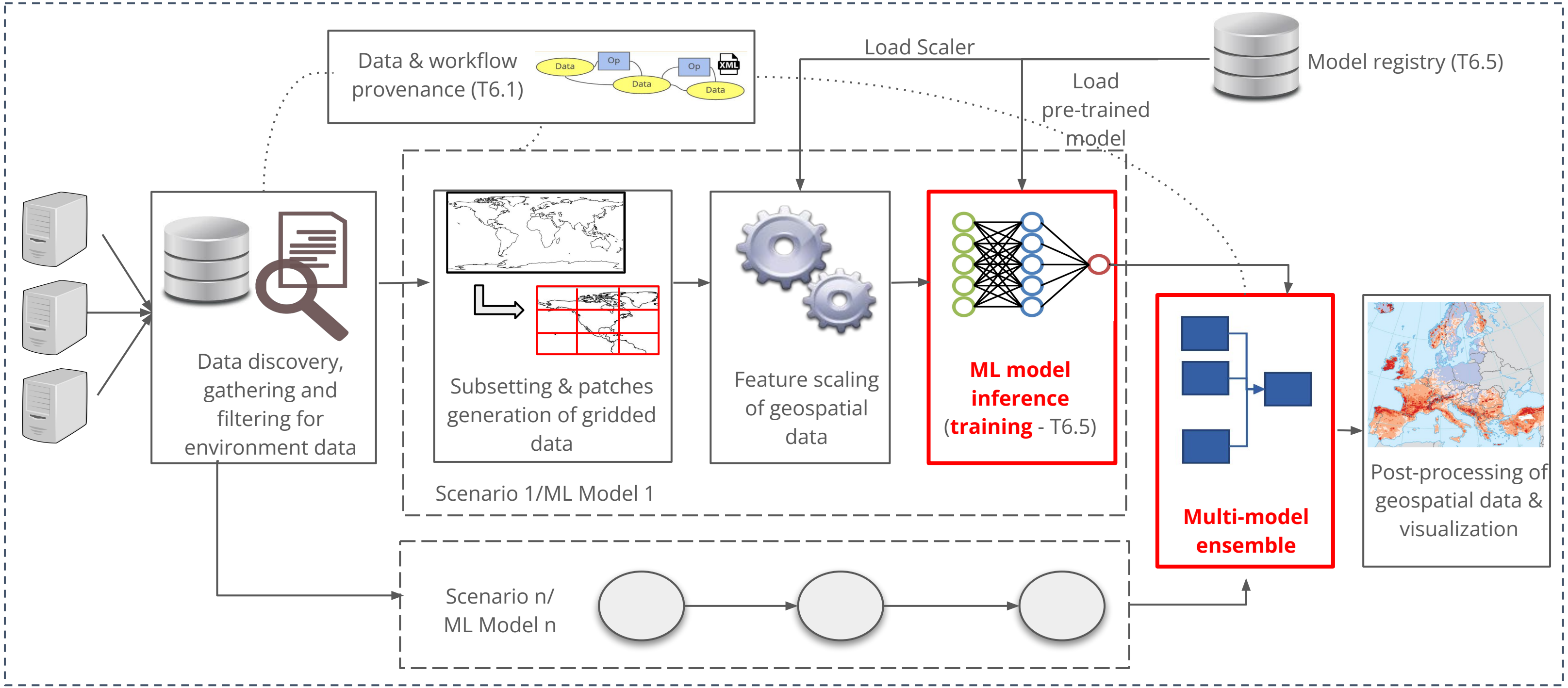
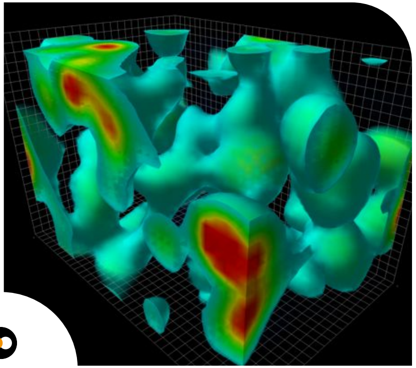

Data & workflow provenance (T6.1)
Data
Op
Data
Op
XML
Data
Load Scaler
Model registry (T6.5)
Load pre-trained model
Data discovery, gathering and filtering for environment data
Subsetting & patches generation of gridded data
Feature scaling of geospatial data
ML model inference (training - T6.5)
Multi-model ensemble
Post-processing of geospatial data & visualization
Scenario 1/ML Model 1
Scenario n/ ML Model n

Image courtesy of Donatello Elia (CMCC)

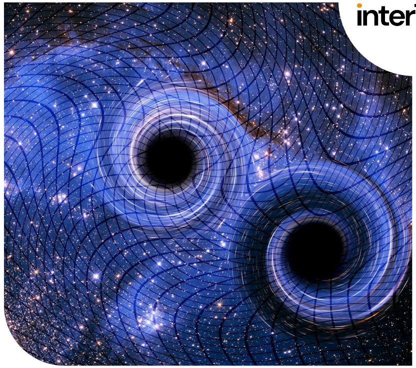
Physics Use Cases in InterTwin

Radio Astronomy
Univ. of Heidelberg,
Max Planck Society

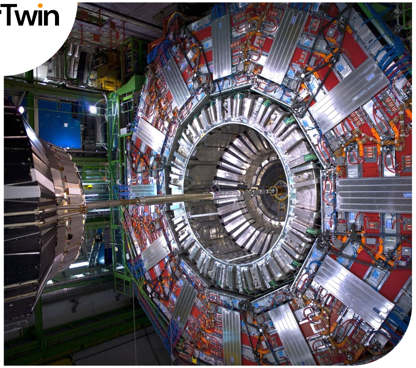
Lattice QCD
CSIC, CNRS



Gravitational Wave Astronomy
INFN



High Energy Physics
CERN, CNRS



DT of Particle Detector

Detector Prototyping & Optimization

Build data-driven tool that **simulates detector response** and integrates operation conditions from experimental setups (test-beams).

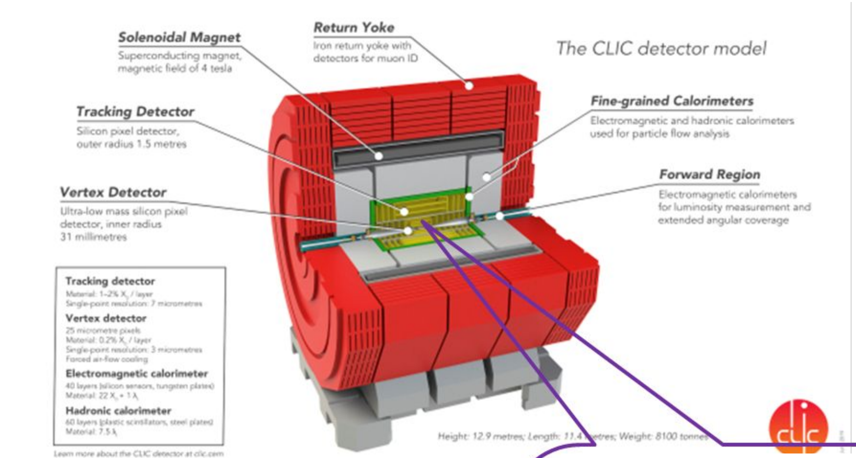
Online ML for Detectors

Adapt **real-time** detector and/or data acquisition configuration with respect to run conditions

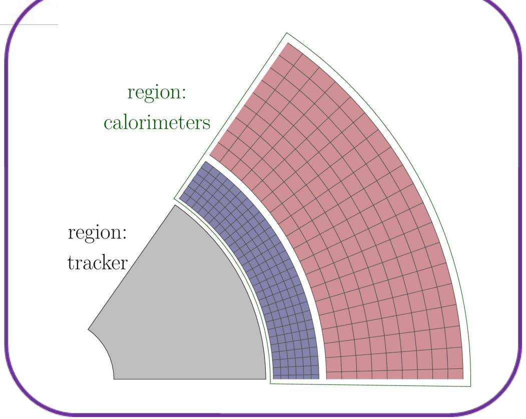
Quality verification & Validation frameworks

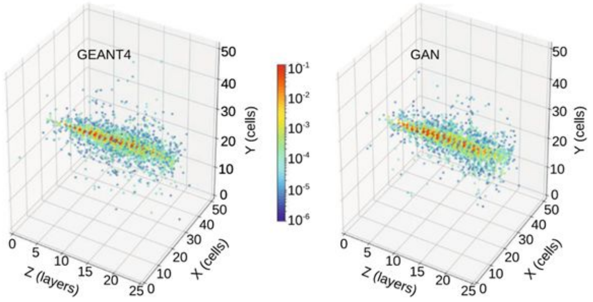
Model convergence and accuracy of the generated data should be monitored.

Development of sample-based validation framework in collaboration with HEP community.



The CLIC detector model
Solenoidal Magnet
Superconducting magnet, magnetic field of 4 tesla
Return Yoke
Iron return yoke with detectors for muon ID
Tracking Detector
Silicon pixel detector, outer radius 1.5 metres
Fine-grained Calorimeters
Electromagnetic and hadronic calorimeters used for particle flow analysis
Vertex Detector
Ultra-low mass silicon pixel detector, inner radius 31 millimetres
Forward Region
Electromagnetic calorimeters for luminosity measurement and extended angular coverage
Tracking detector
Material: 1–2% X0 / layer
Single-point resolution: 7 micrometres
Vertex detector
25 micrometre pixels
Material: 0.2% X0 / layer
Single-point resolution: 3 micrometres
Forced air-flow cooling
Electromagnetic calorimeter
40 layers (silicon sensors, tungsten plates)
Material: 22 X0 + 1 λI
Hadronic calorimeter
60 layers (plastic scintillators, steel plates)
Material: 7.5 λI
Height: 12.9 metres; Length: 11.4 metres; Weight: 8100 tonnes
Learn more about the CLIC detector at clic.cern





Fast Simulation of a High Granularity Calorimeter by Generative Adversarial Networks. Gul Rukh Khattak et al. https://arxiv.org/abs/2109.07388 DOI: https://doi.org/10.48550/arXiv.2109.07388

interTwin

Benefits of interdisciplinary approach

- **Collaboration**: Increase in cross-community development efforts and unification of frameworks used - “breaking down silos”.

- **Portability**: Run DT workflows infrastructure agnostic across multiple HPC centers in Europe.

- **Extensibility**: Easy addition of new use cases.

- **Modularity**: Customizable according to specific use case’s needs.

DT Core Engine – ML capabilities

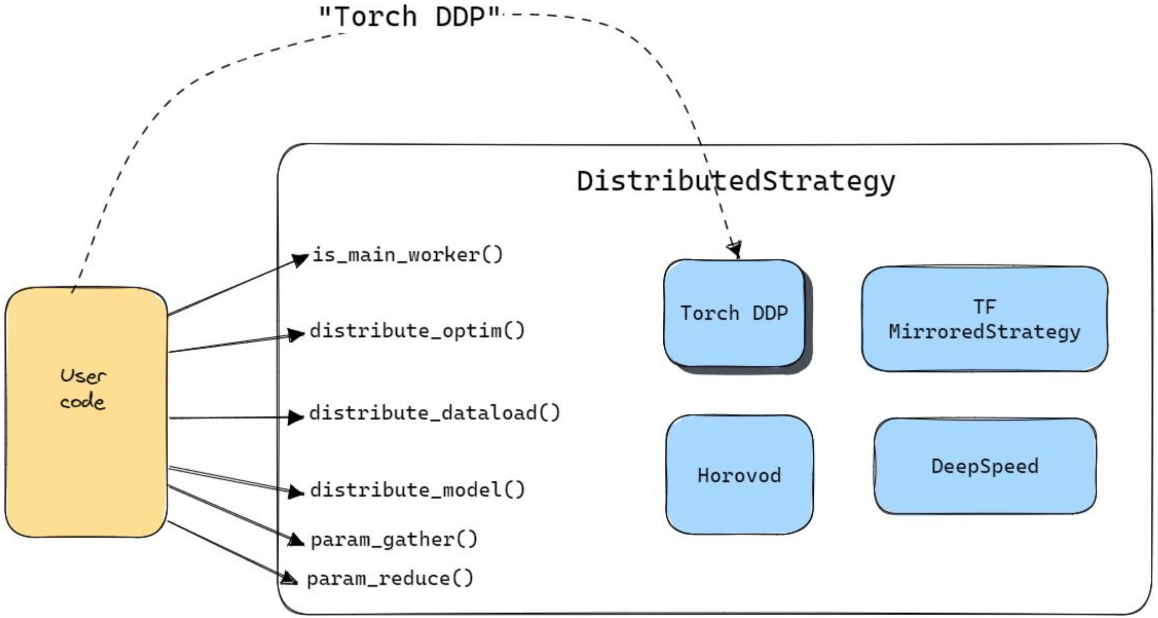
Our contribution to the Core Engine

Support AI-based digital twin applications in science:

- **Reproducibility, Reusability, and Modularity**
- **Framework-independent** (e.g., PyTorch, TensorFlow, XGBoost, MLFlow, WandB)
- **UX/UI**: user-friendly GUI (e.g., JupyterLab)
- Off-the-shelf AI tooling:
  - **Hyper-parameters optimization**
  - Scalability (e.g., **distributed ML**)
  - State of the Art **models repository**
- **Seamless access to infrastructure** (cloud and HPC resources)

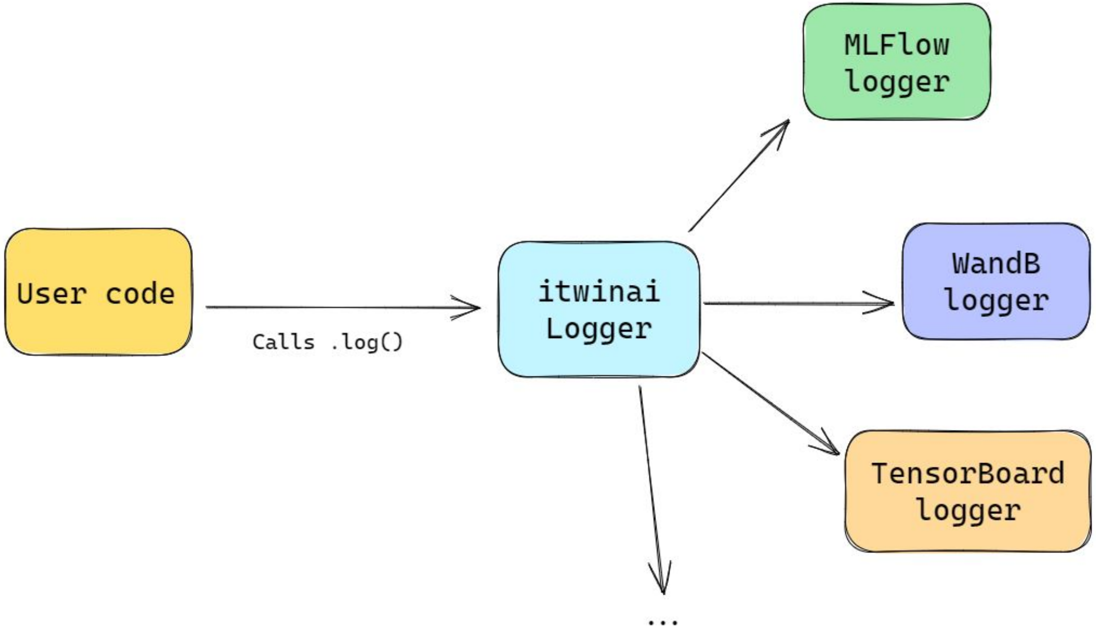
Our contribution to the Core Engine

Unified distributed training (informal representation)

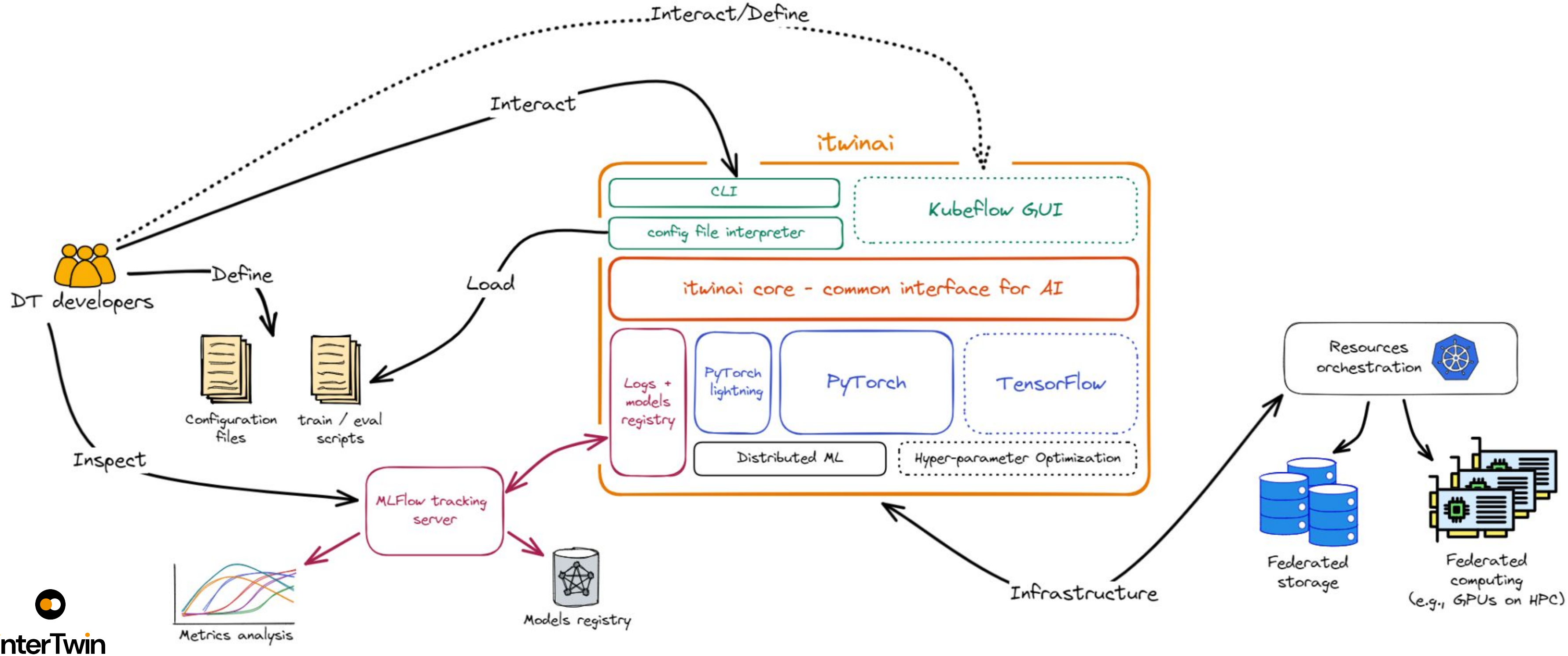


Our contribution to the Core Engine

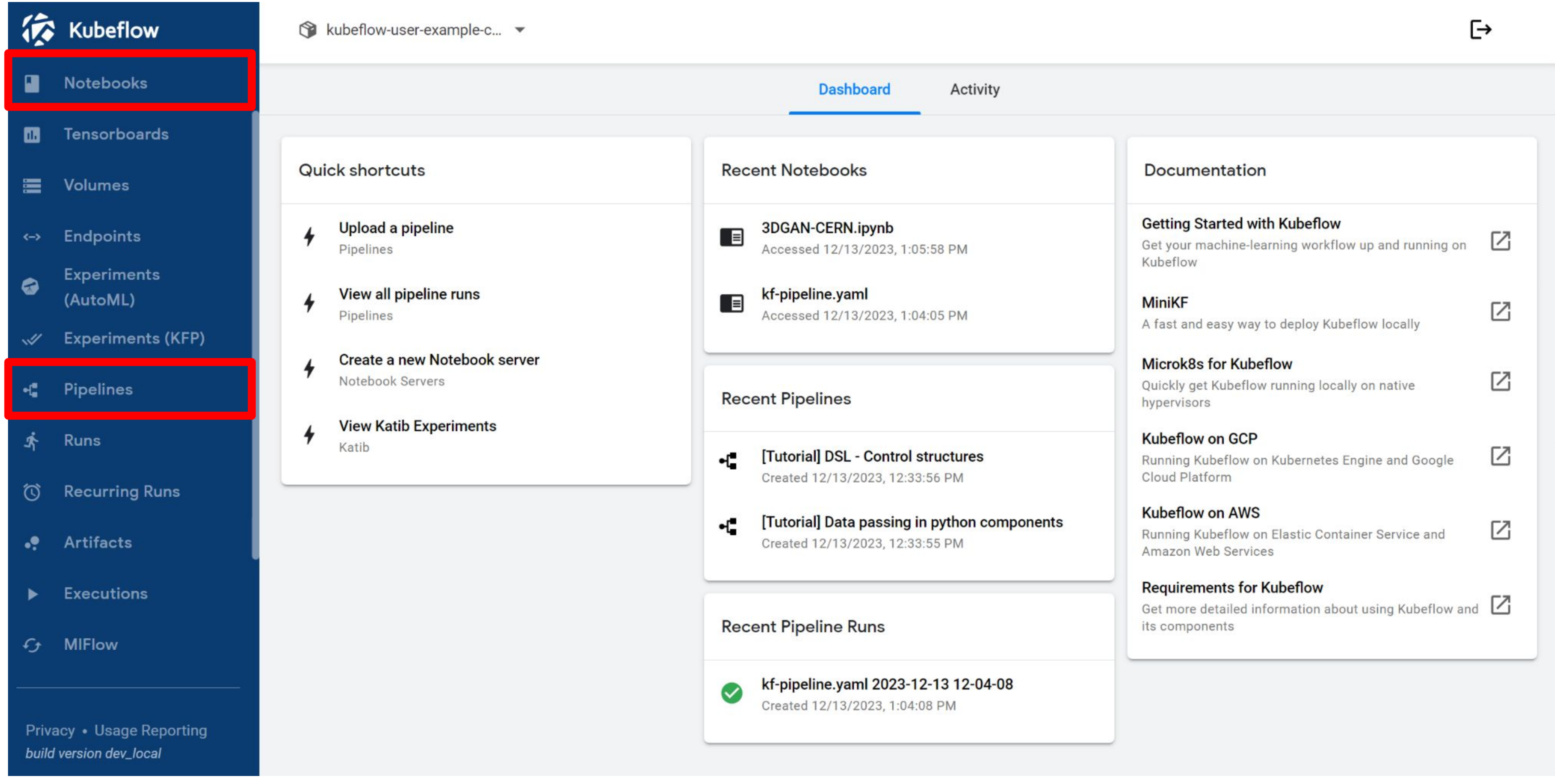
Generic logger (informal representation)



Itwinai - ML tooling for DT applicaitons



UX/UI: KubeFlow



Quick shortcuts

- Upload a pipeline — Pipelines
- View all pipeline runs — Pipelines
- Create a new Notebook server — Notebook Servers
- View Katib Experiments — Katib

Recent Notebooks

- 3DGAN-CERN.ipynb — Accessed 12/13/2023, 1:05:58 PM
- kf-pipeline.yaml — Accessed 12/13/2023, 1:04:05 PM

Recent Pipelines

- [Tutorial] DSL - Control structures — Created 12/13/2023, 12:33:56 PM
- [Tutorial] Data passing in python components — Created 12/13/2023, 12:33:55 PM

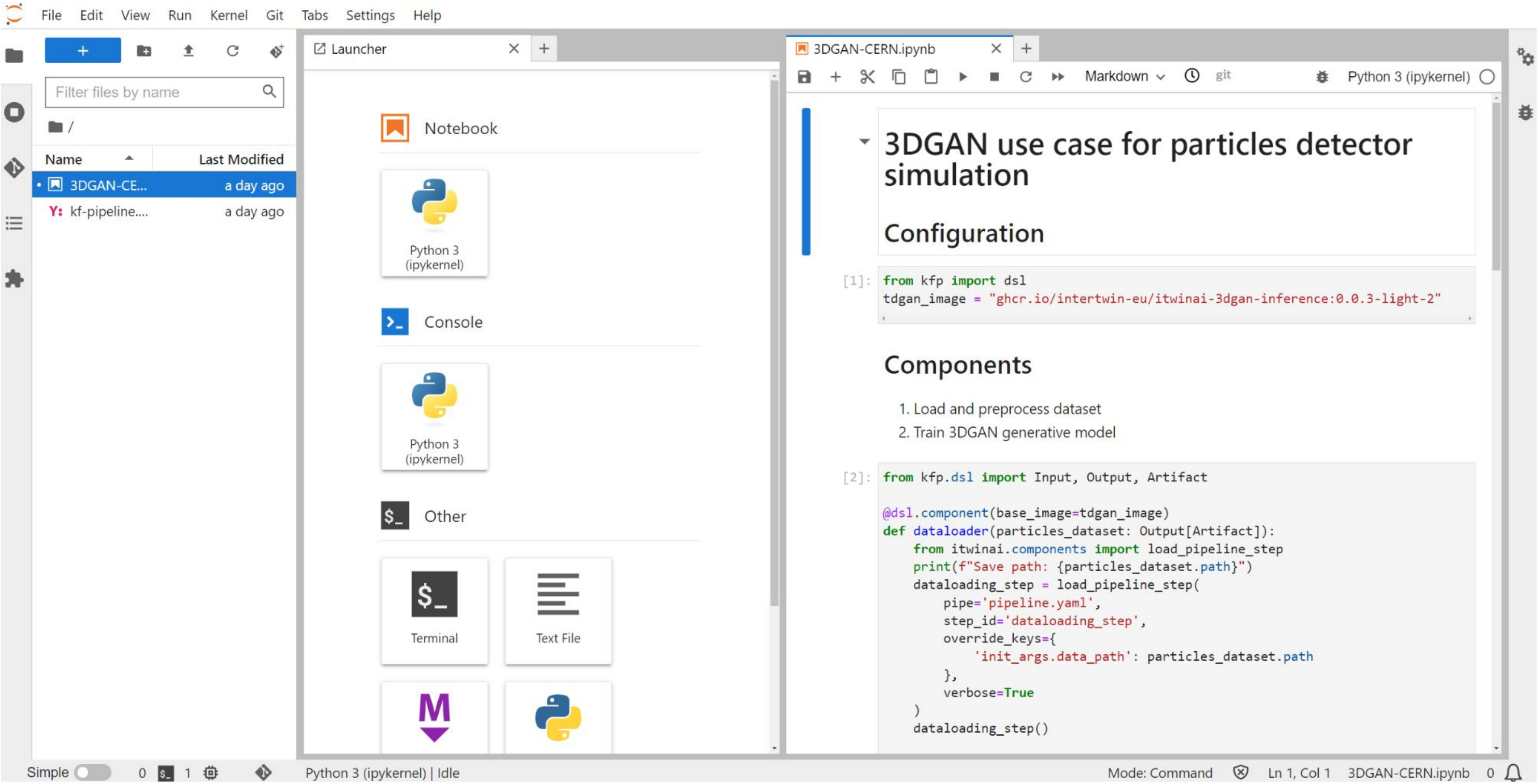
Recent Pipeline Runs

- kf-pipeline.yaml 2023-12-13 12-04-08 — Created 12/13/2023, 1:04:08 PM

Documentation

- Getting Started with Kubeflow — Get your machine-learning workflow up and running on Kubeflow
- MiniKF — A fast and easy way to deploy Kubeflow locally
- Microk8s for Kubeflow — Quickly get Kubeflow running locally on native hypervisors
- Kubeflow on GCP — Running Kubeflow on Kubernetes Engine and Google Cloud Platform
- Kubeflow on AWS — Running Kubeflow on Elastic Container Service and Amazon Web Services
- Requirements for Kubeflow — Get more detailed information about using Kubeflow and its components

UX/UI: KubeFlow and JupyterLab



3DGAN use case for particles detector simulation

Configuration

```
[1]: from kfp import dsl
     tdgan_image = "ghcr.io/intertwin-eu/itwinai-3dgan-inference:0.0.3-light-2"
```

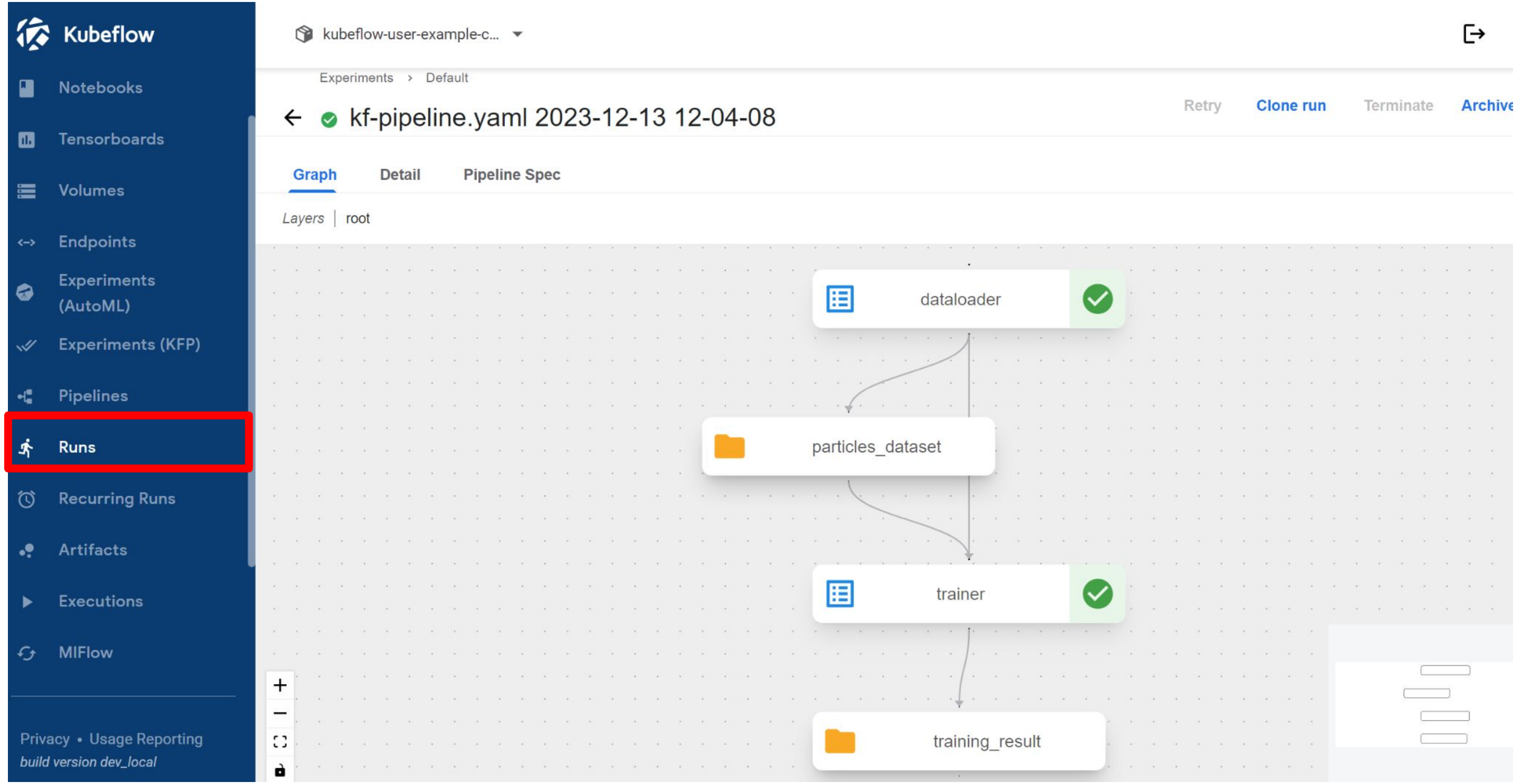
Components

1. Load and preprocess dataset
2. Train 3DGAN generative model

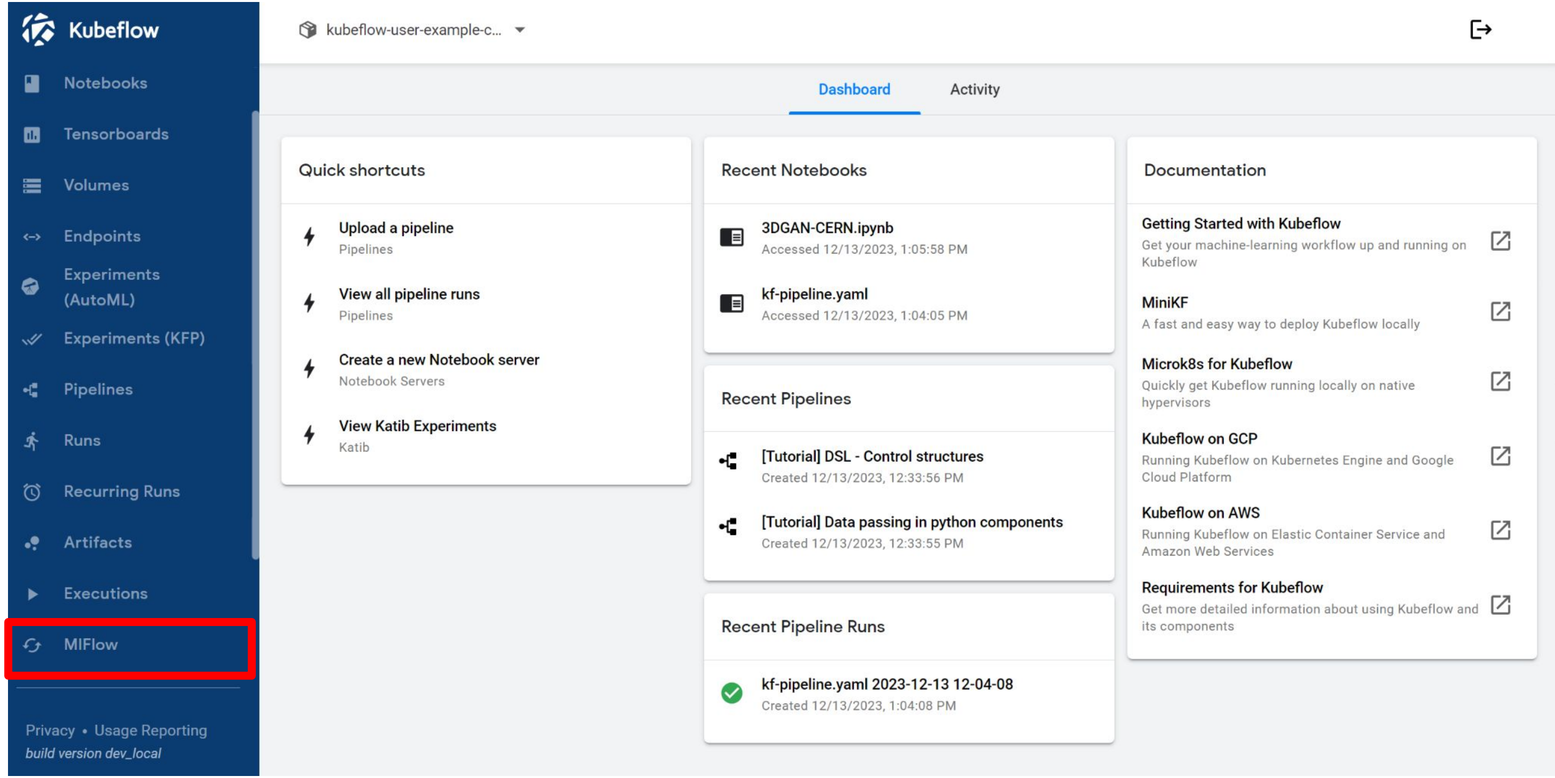
```
[2]: from kfp.dsl import Input, Output, Artifact

     @dsl.component(base_image=tdgan_image)
     def dataloader(particles_dataset: Output[Artifact]):
         from itwinai.components import load_pipeline_step
         print(f"Save path: {particles_dataset.path}")
         dataloading_step = load_pipeline_step(
             pipe='pipeline.yaml',
             step_id='dataloading_step',
             override_keys={
                 'init_args.data_path': particles_dataset.path
             },
             verbose=True
         )
         dataloading_step()
```

UX/UI: KubeFlow pipelines



UX/UI: KubeFlow and MLFlow



Quick shortcuts

- Upload a pipeline
  Pipelines
- View all pipeline runs
  Pipelines
- Create a new Notebook server
  Notebook Servers
- View Katib Experiments
  Katib

Recent Notebooks

- 3DGAN-CERN.ipynb
  Accessed 12/13/2023, 1:05:58 PM
- kf-pipeline.yaml
  Accessed 12/13/2023, 1:04:05 PM

Recent Pipelines

- [Tutorial] DSL - Control structures
  Created 12/13/2023, 12:33:56 PM
- [Tutorial] Data passing in python components
  Created 12/13/2023, 12:33:55 PM

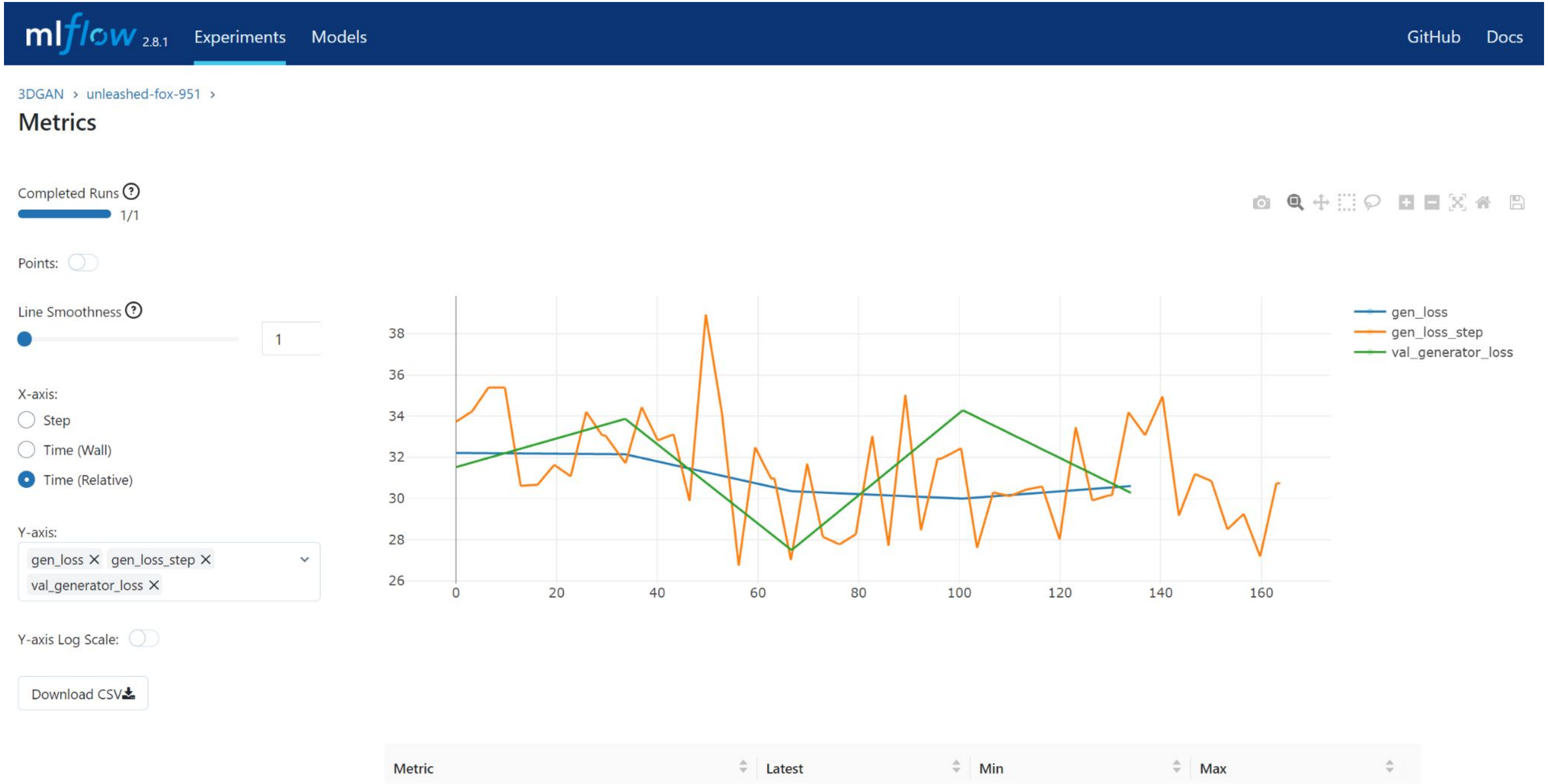
Recent Pipeline Runs

- ✓ kf-pipeline.yaml 2023-12-13 12-04-08
  Created 12/13/2023, 1:04:08 PM

Documentation

- Getting Started with Kubeflow
  Get your machine-learning workflow up and running on Kubeflow
- MiniKF
  A fast and easy way to deploy Kubeflow locally
- Microk8s for Kubeflow
  Quickly get Kubeflow running locally on native hypervisors
- Kubeflow on GCP
  Running Kubeflow on Kubernetes Engine and Google Cloud Platform
- Kubeflow on AWS
  Running Kubeflow on Elastic Container Service and Amazon Web Services
- Requirements for Kubeflow
  Get more detailed information about using Kubeflow and its components

UX/UI: MLFlow logs



3DGAN › unleashed-fox-951 ›

Metrics

Completed Runs ? 1/1

Points: ○

Line Smoothness ? 1

X-axis:

○ Step

○ Time (Wall)

● Time (Relative)

Y-axis:

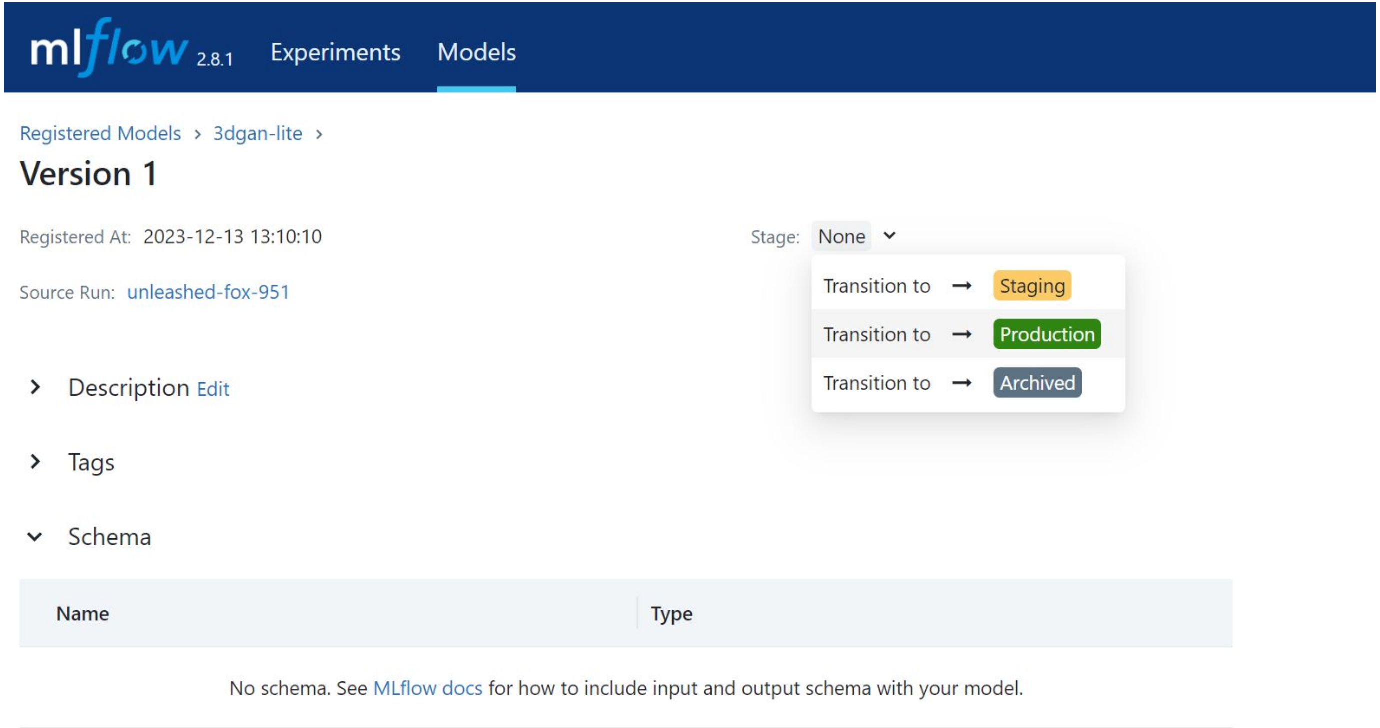
gen_loss ✕ gen_loss_step ✕ val_generator_loss ✕

Y-axis Log Scale: ○

Download CSV

Metric	Latest	Min	Max

UX/UI: MLFlow models registry



Registered Models › 3dgan-lite ›

Version 1

Registered At: 2023-12-13 13:10:10

Source Run: unleashed-fox-951

Stage: None

› Description Edit

› Tags

⌄ Schema

Name	Type

No schema. See MLflow docs for how to include input and output schema with your model.

Latest news

Development status of itwinai library:

- Support for **PyTorch**, investigation towards **TensorFlow**
- **AI workflows**: exploration of **KubeFlow** Pipelines.
- **Distributed ML**: integration of existing strategies (e.g., DDP, Horovod, DeepSpeed)..
- **Link with the infrastructure**: Docker/Singularity container, offloaded through WP5's **interLink** on cloud/HPC systems.
- **ML logs and models**: MLFlow tracking

Demo time

Demo video: https://www.youtube.com/watch?v=NoVCfSxwtX0

GitHub repository: https://github.com/interTwin-eu/itwinai

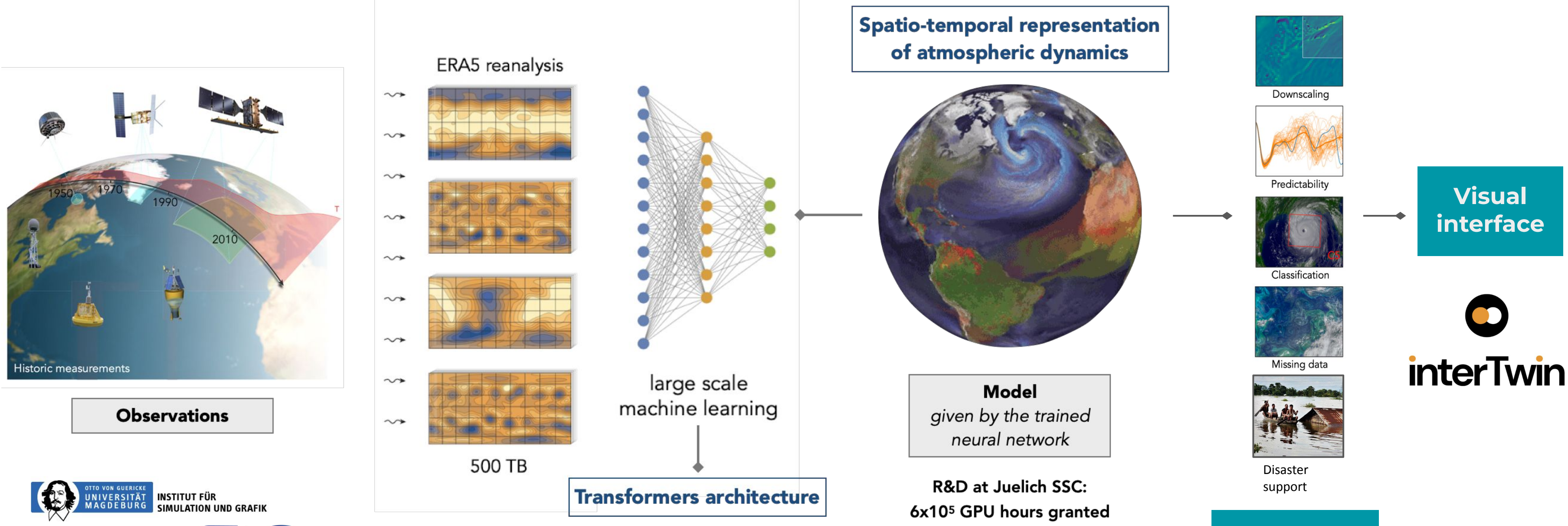
- For the moment, please refer to the "dev" branch: https://github.com/interTwin-eu/itwinai/tree/dev
- Some **tutorials** available, **more to come**. Check "tutorials" folder: https://github.com/interTwin-eu/itwinai/tree/dev/tutorials
- Additional examples are under "use-cases" folder: https://github.com/interTwin-eu/itwinai/tree/dev/use-cases

interTwin

Other DT initiatives

EMP^2: Environmental Modelling and prediction platform

First proof-of-concept of a machine-learning based global environmental model trained on terabytes of observational data



Observations

Transformers architecture

Spatio-temporal representation of atmospheric dynamics

Model
given by the trained neural network

R&D at Juelich SSC:
6x10^5 GPU hours granted in 2022

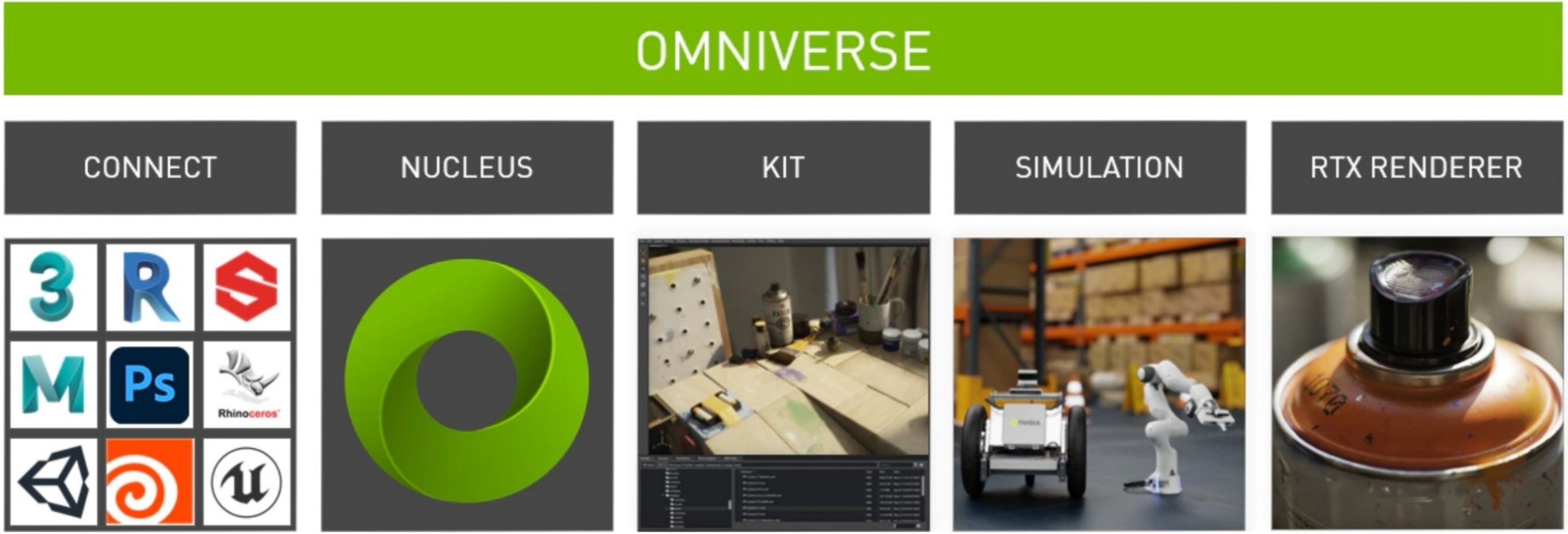
Applications

Visual interface

OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG INSTITUT FÜR SIMULATION UND GRAFIK
JÜLICH Forschungszentrum
CERN | CIPEA CERN Innovation Programme on Environmental Applications

Slide courtesy of Ilaria Luise

Nvidia Omniverse (OV)


OMNIVERSE

CONNECT

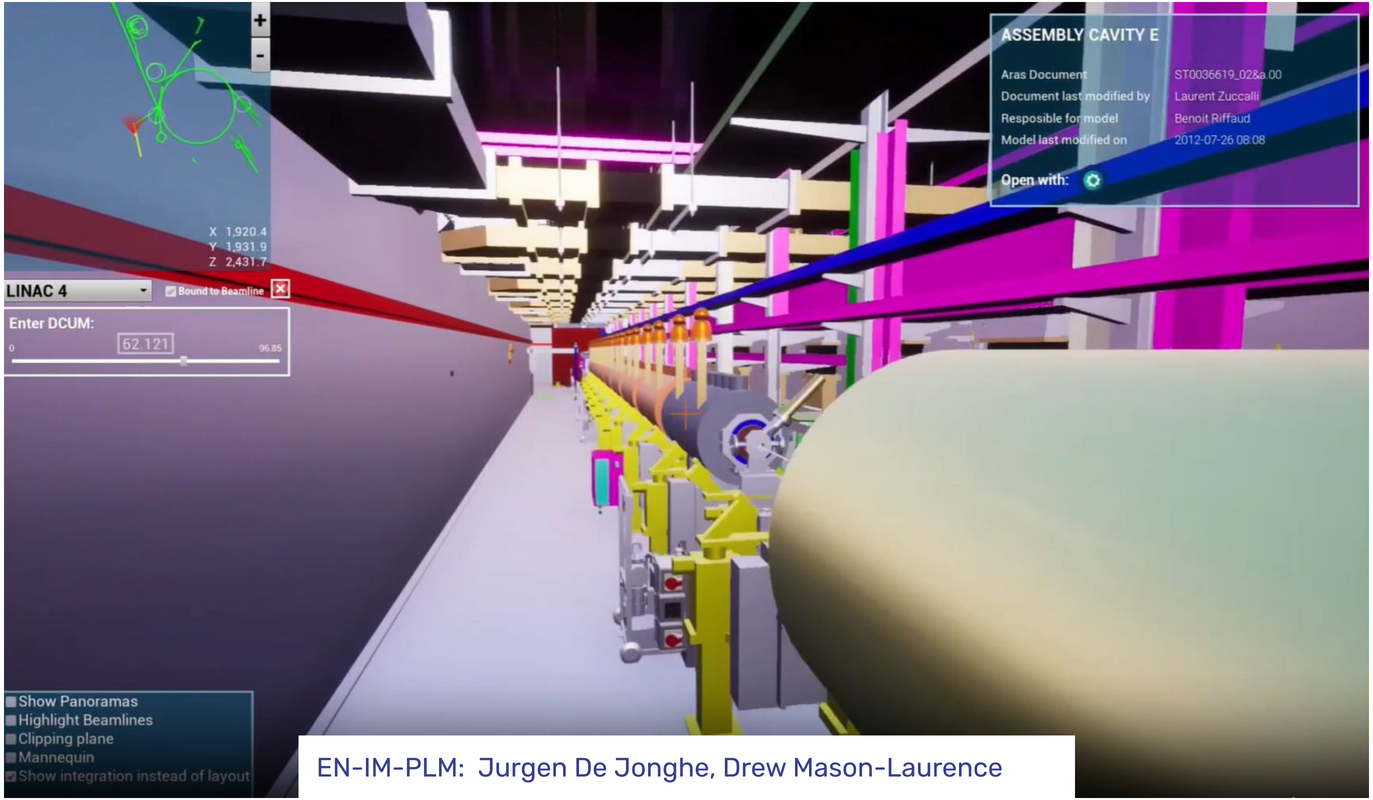
NUCLEUS

KIT

SIMULATION

RTX RENDERER

OV for DTs of the accelerators complex



ASSEMBLY CAVITY E

Aras Document ST0036619_02&a.00

Document last modified by Laurent Zuccalli

Resposible for model Benoit Riffaud

Model last modified on 2012-07-26 08:08

Open with:

X 1,920.4
Y 1,931.9
Z 2,431.7

LINAC 4

☑ Bound to Beamline

Enter DCUM: 62.121

■ Show Panoramas
■ Highlight Beamlines
■ Clipping plane
■ Mannequin
☑ Show integration instead of layout

EN-IM-PLM: Jurgen De Jonghe, Drew Mason-Laurence

Nvidia Omniverse - Opportunities

- Detector assembly simulation

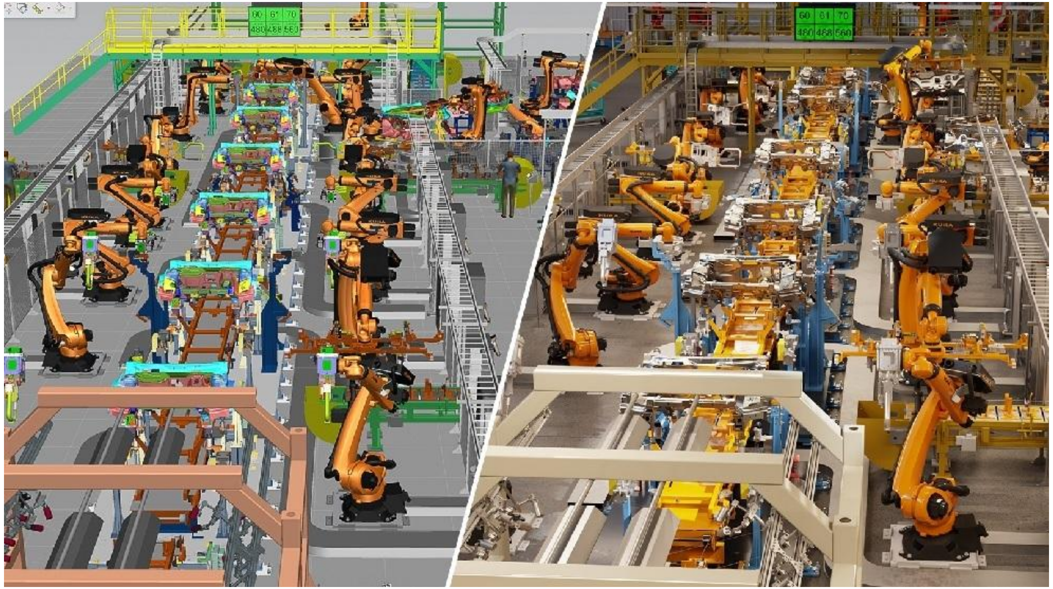


Image credits: https://blogs.sw.siemens.com/thought-leadership/2022/06/29/creating-the-industrial-metaverse-siemens-xcelerator-nvidia-omniverse/

Nvidia Omniverse - Opportunities

- Robotic simulation. IsaacGym can also train Reinforcement learning agents.

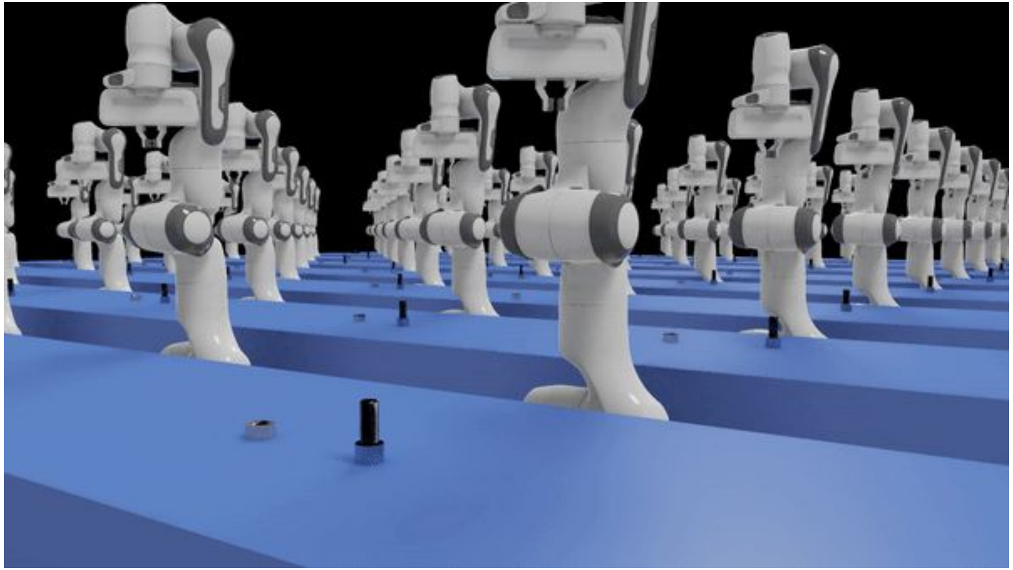


Image credits: https://developer.nvidia.com/blog/advancing-robotic-assembly-with-a-novel-simulation-approach-using-nvidia-isaac/

See also: https://github.com/NVIDIA-Omniverse/OmniIsaacGymEnvs

Nvidia Omniverse - Opportunities

- Visualizations for HEP with Geant4

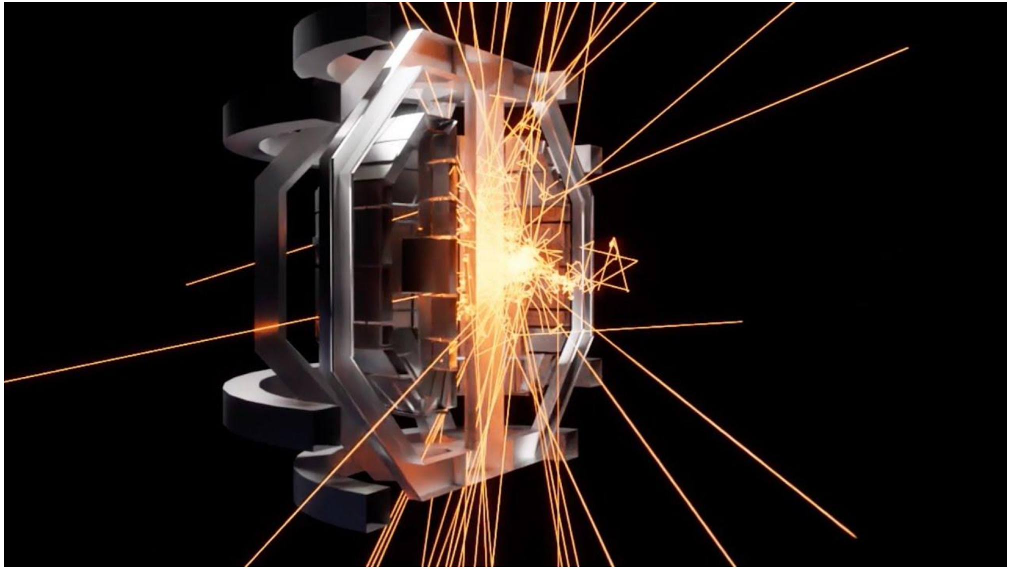


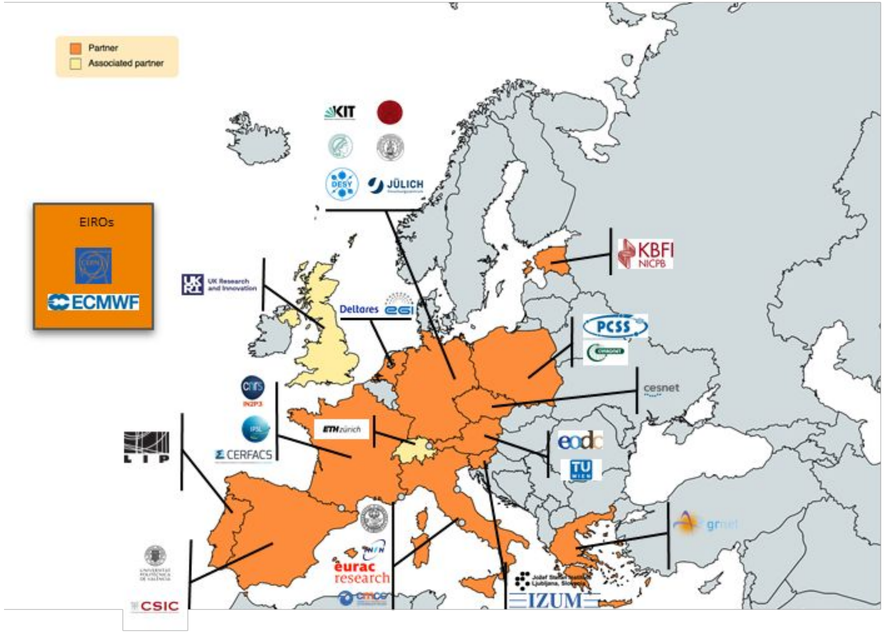
Image credits: https://blogs.nvidia.com/blog/ukaea-digital-twins-omniverse/

CERN openlab

Digital Twin Engine

A focus on the architecture

interTwin consortium



EGI Foundation as coordinator

29 **Participants**, including 1 affiliated entity and 2 associated partners

Consortium at a glance

10
Providers

cloud, HTC , HPC resources and access to Quantum systems

11
Technology providers

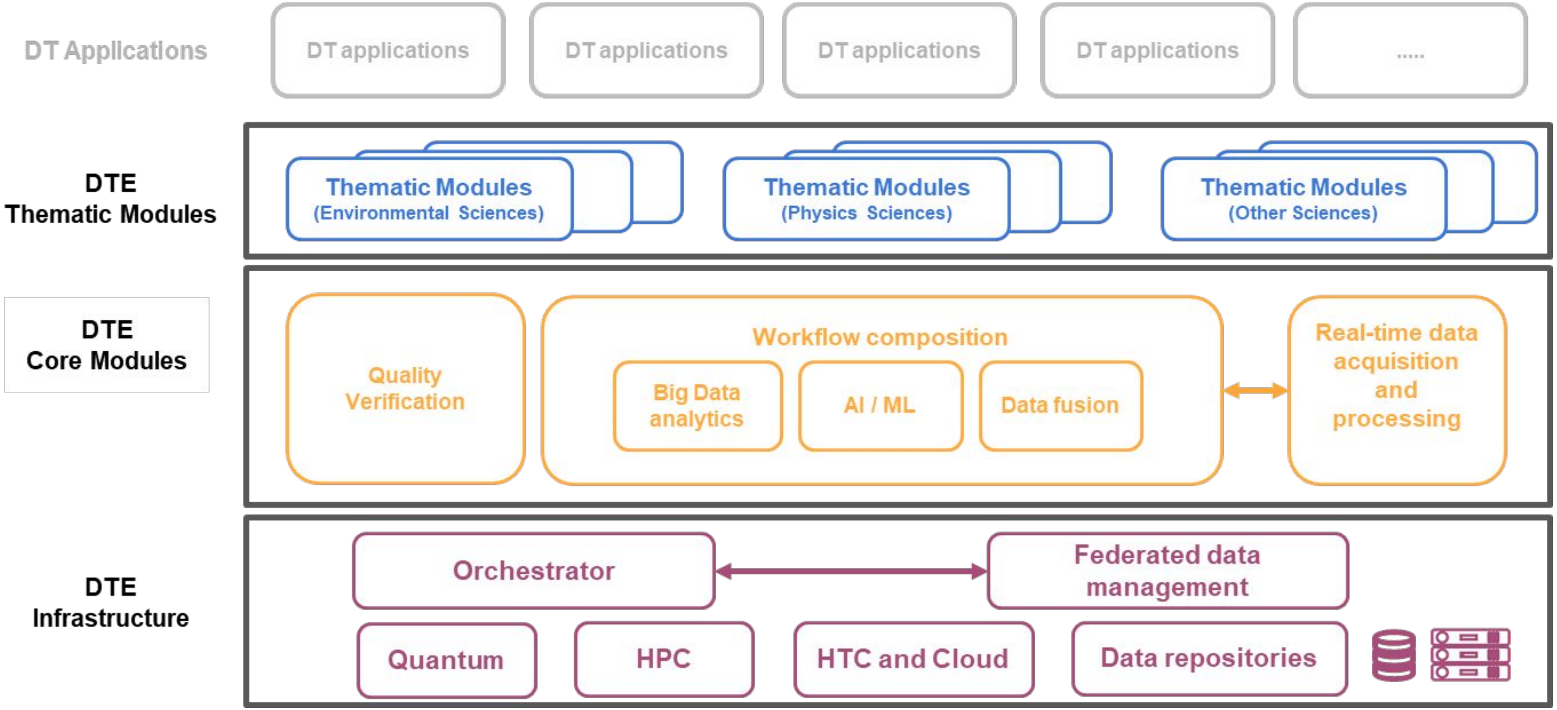
delivering the DTE infrastructure and horizontal capabilities

14
Community representatives

from 5 scientific areas; requirements and developing DT applications and thematic modules

interTwin

interTwin - DT Engine stack



DT Engine for science

Today

- DTs developed in isolation
- Community-specific technologies and standards
- **Great overheads** (i.e., reinventing the wheel)

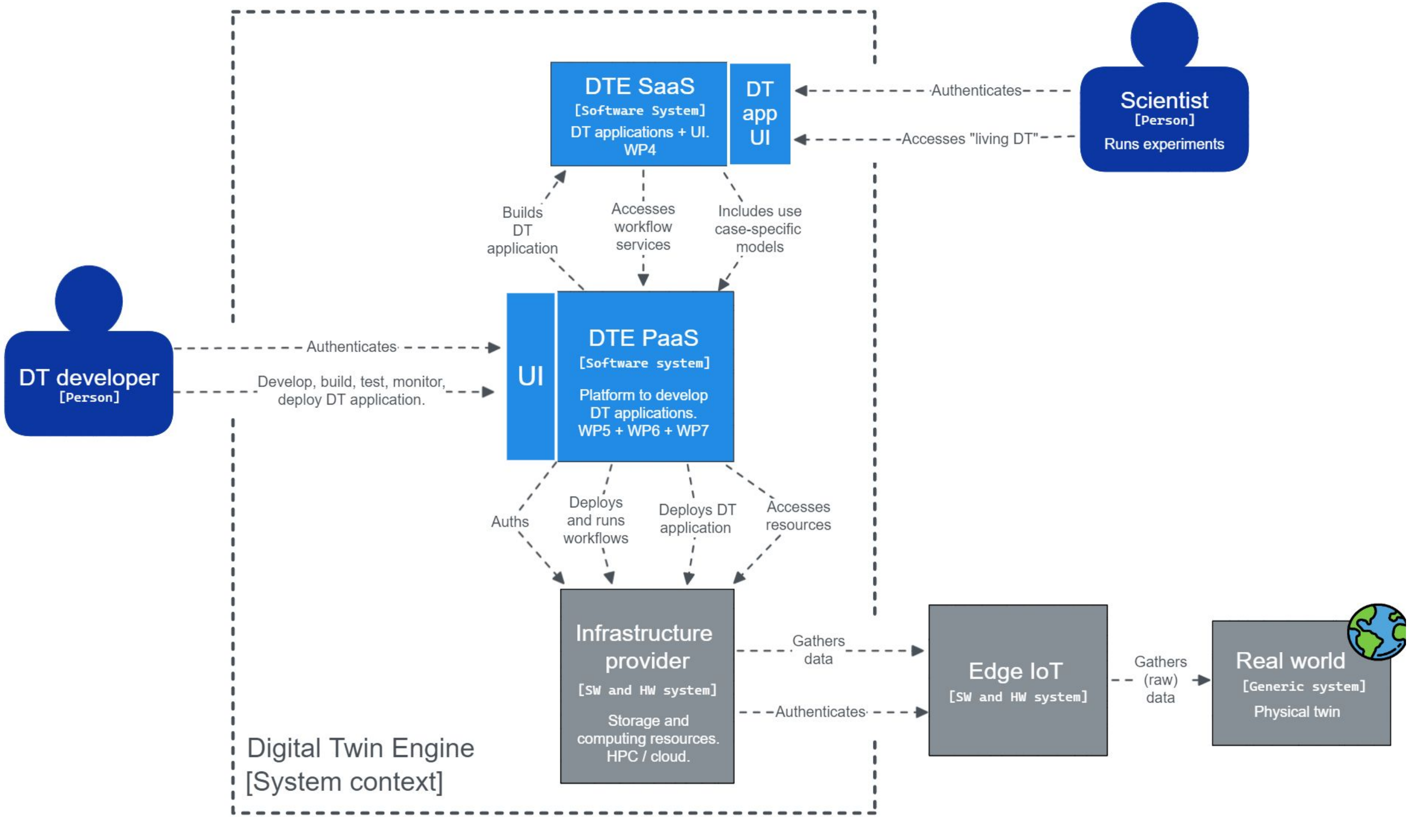
Boils down to… **need for improvement.**

Tomorrow

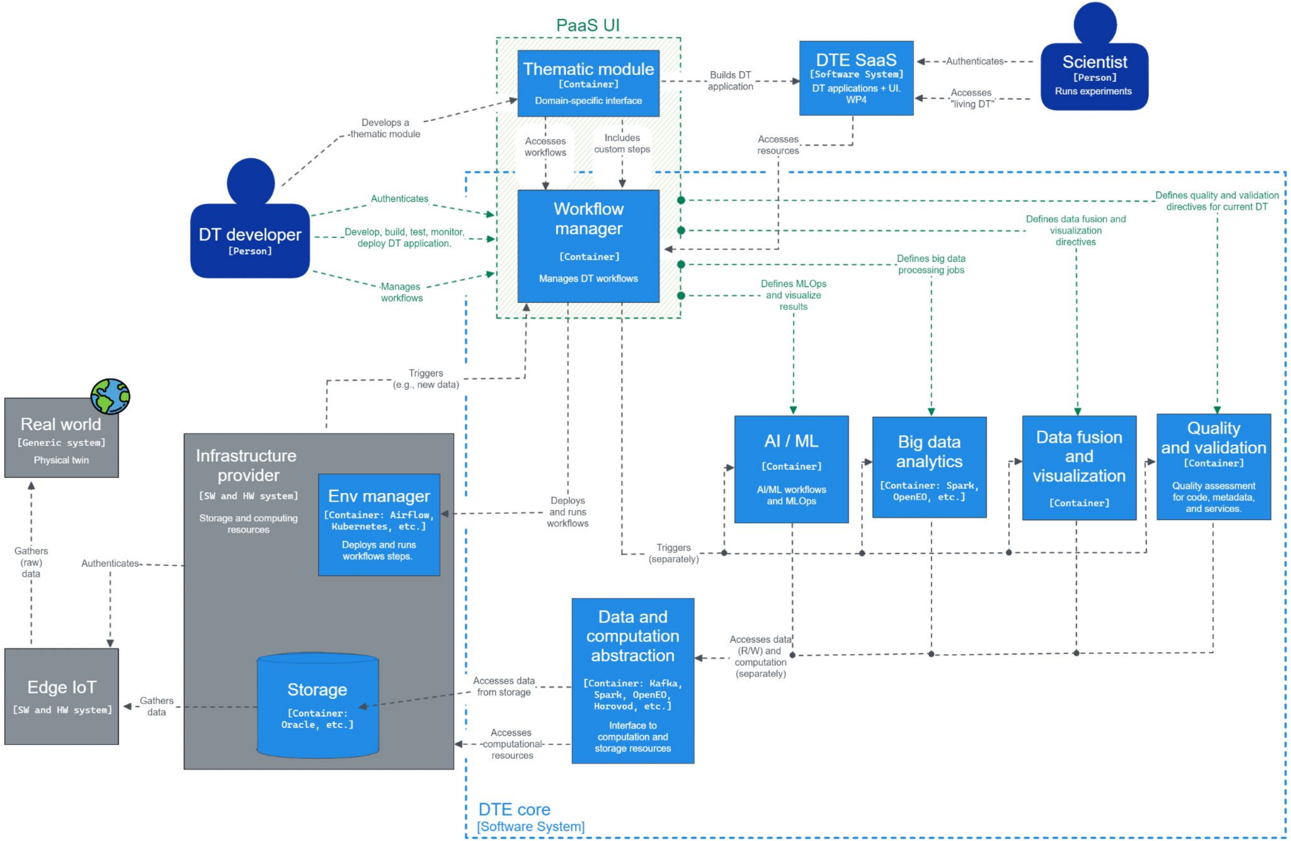
- Unified DTE framework
- Standard DT lifecycle management, thanks to co-design
- **Low overheads** (engineering)

Results into… **accelerated science!**

Digital twin engine - System context

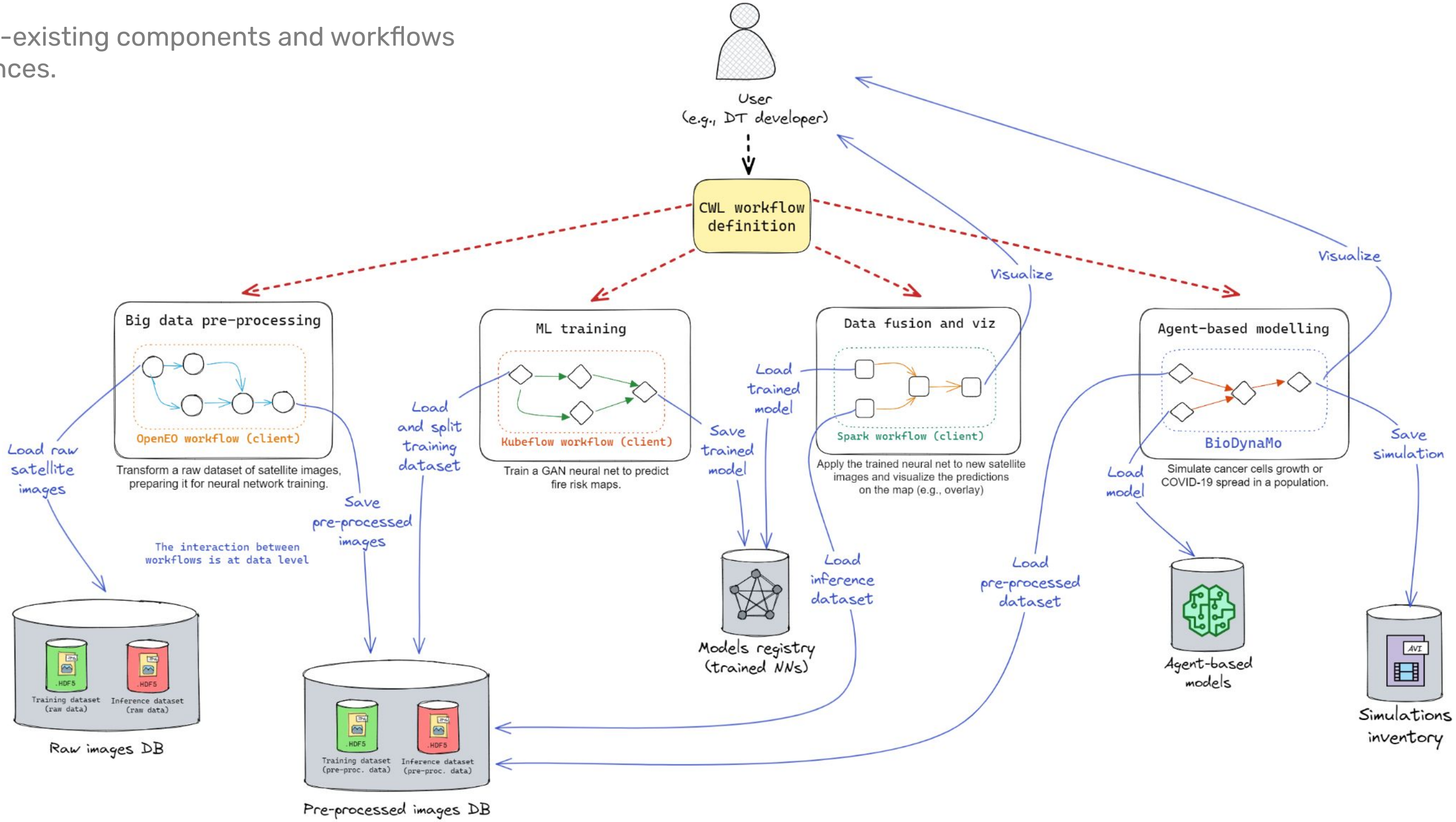


Digital twin engine - DT workflows


PaaS UI
Thematic module
[Container]
Domain-specific interface
Builds DT application
DTE SaaS
[Software System]
DT applications + UI. WP4
Authenticates
Accesses "living DT"
Scientist
[Person]
Runs experiments
Develops a thematic module
Accesses workflows
Includes custom steps
Accesses resources
DT developer
[Person]
Authenticates
Develop, build, test, monitor, deploy DT application.
Manages workflows
Workflow manager
[Container]
Manages DT workflows
Defines quality and validation directives for current DT
Defines data fusion and visualization directives
Defines big data processing jobs
Defines MLOps and visualize results
Triggers (e.g., new data)
Real world
[Generic system]
Physical twin
Infrastructure provider
[SW and HW system]
Storage and computing resources
Env manager
[Container: Airflow, Kubernetes, etc.]
Deploys and runs workflows steps.
Deploys and runs workflows
AI / ML
[Container]
AI/ML workflows and MLOps
Big data analytics
[Container: Spark, OpenEO, etc.]
Data fusion and visualization
[Container]
Quality and validation
[Container]
Quality assessment for code, metadata, and services.
Triggers (separately)
Gathers (raw) data
Authenticates
Data and computation abstraction
[Container: Kafka, Spark, OpenEO, Horovod, etc.]
Interface to computation and storage resources
Accesses data (R/W) and computation (separately)
Edge IoT
[SW and HW system]
Gathers data
Storage
[Container: Oracle, etc.]
Accesses data from storage
Accesses computational resources
DTE core
[Software System]

Use case-specific components

Reuse pre-existing components and workflows from sciences.



CWL workflow definition

Big data pre-processing

OpenEO workflow (client)

Transform a raw dataset of satellite images, preparing it for neural network training.

ML training

Kubeflow workflow (client)

Train a GAN neural net to predict fire risk maps.

Data fusion and viz

Spark workflow (client)

Apply the trained neural net to new satellite images and visualize the predictions on the map (e.g., overlay)

Agent-based modelling

BioDynaMo

Simulate cancer cells growth or COVID-19 spread in a population.

The interaction between workflows is at data level

User
(e.g., DT developer)
Visualize
Visualize
Load raw satellite images
Save pre-processed images
Load and split training dataset
Save trained model
Load trained model
Load inference dataset
Load pre-processed dataset
Load model
Save simulation
.HDF5
Training dataset (raw data)
.HDF5
Inference dataset (raw data)
Raw images DB
.HDF5
Training dataset (pre-proc. data)
.HDF5
Inference dataset (pre-proc. data)
Pre-processed images DB
Models registry (trained NNs)
Agent-based models
AVI
Simulations inventory