interTwin project – CERN openlab use case

CERN openlab summer student lecture, 29 July 2024

Kalliopi Tsolaki, Matteo Bunino, Maria Girone, Alberto Di Meglio, Sofia Vallecorsa, CERN-IT

Funded by the European Union

The interTwin project is funded by the European Union - Grant Agreement Number 101058386

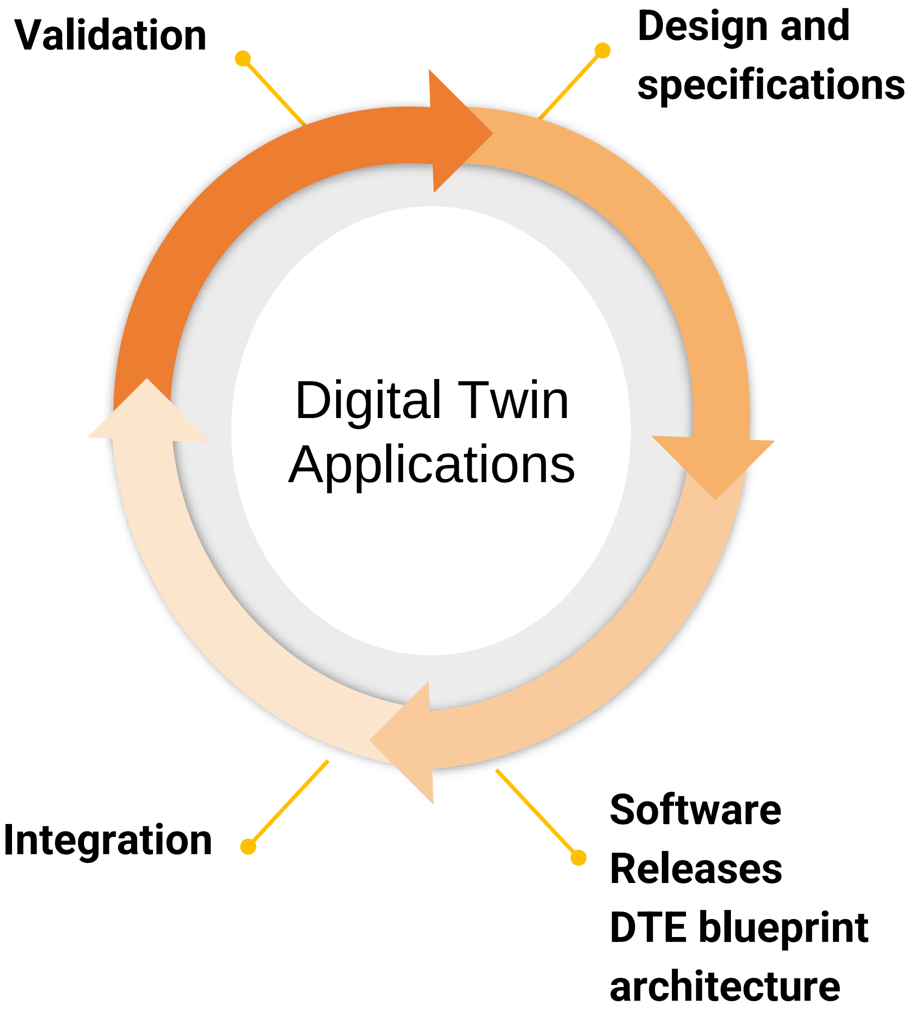
interTwin - Digital Twin Engine for science

A **Digital Twin (DT)** is a **virtual** representation of a **physical** object, process, or system. It is created and sustained with information derived from one or many sources of data such as sensors or models considering historical as well as real-time observations.

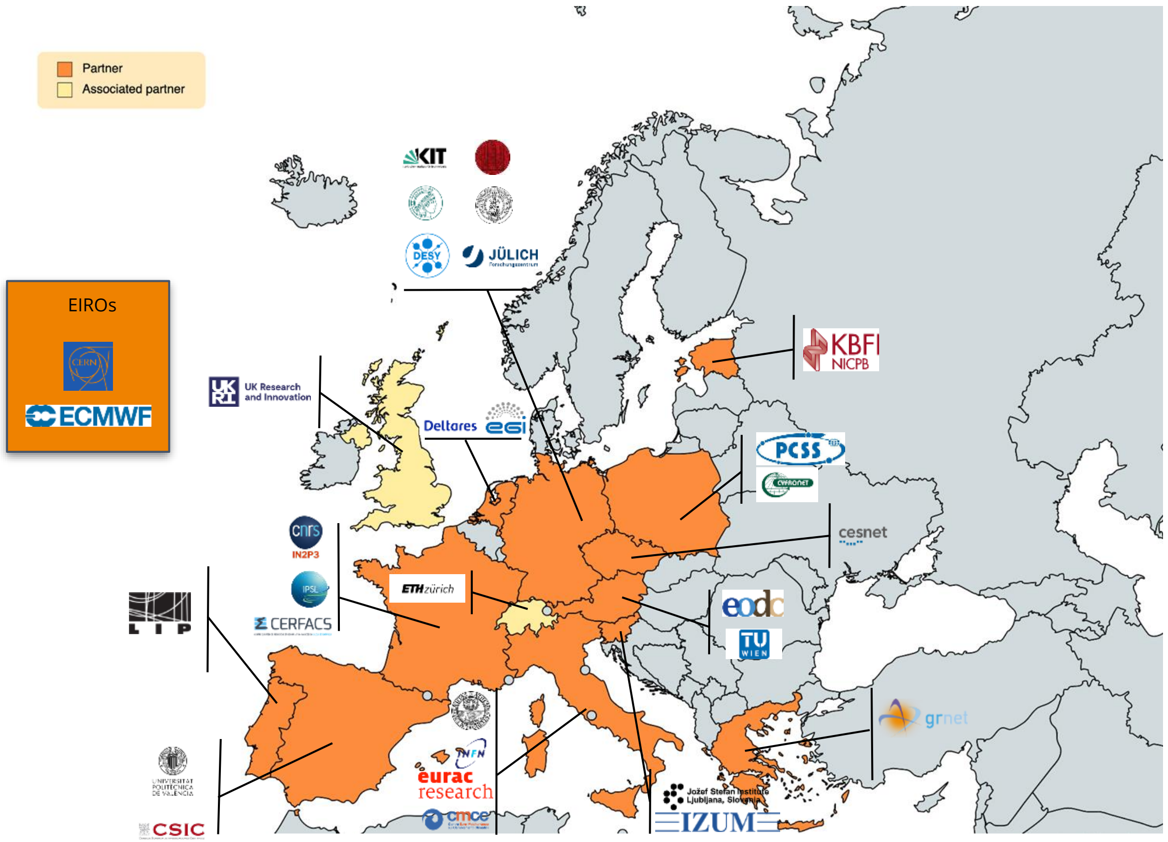
Co-design and implement the prototype of an **interdisciplinary Digital Twin Engine**

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

Large spectrum of **diverse use cases** from **physics** and **environment** sciences



interTwin Consortium

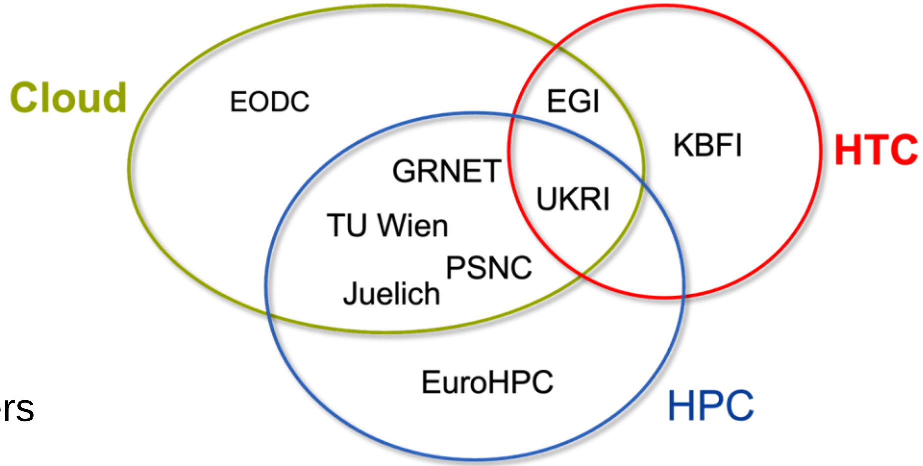


1.09.22 - 31.08.25

Coordinator: EGI

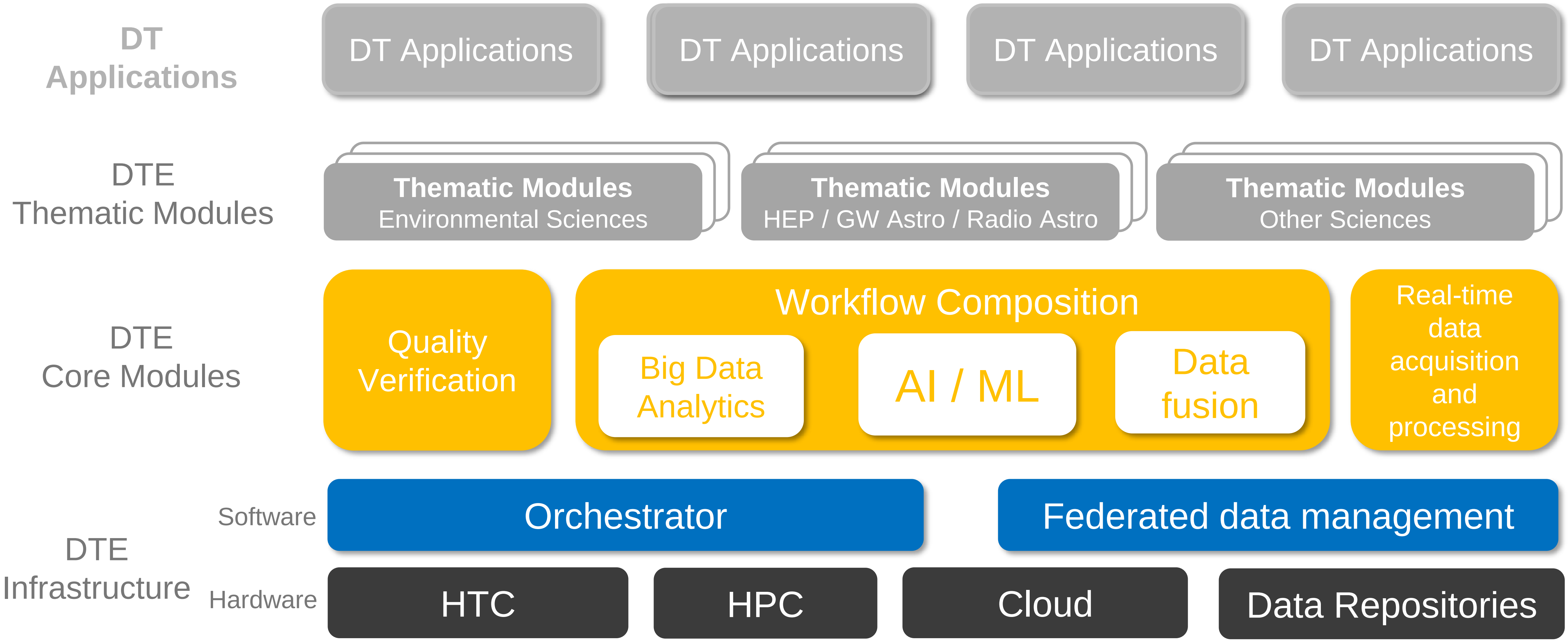
30

Participants,
1 affiliated entity
2 associated partners



10 Providers	11 Technology providers	14 Community representants
Resources: **Cloud** **HTC** **HPC**	delivering the DTE infrastructure and horizontal capabilities	from 5 domains requirements and developing DT applications

interTwin Components



interTwin use cases

Early warning for Extreme events
Deltares, EURAC, TU Wien

WildFire Hazard Map Generation
CMCC, CNRS, Univ. of Trento

Tropical Cyclone Detection
CMCC, CNRS, Univ. of Trento

Extreme events impacts
CERFACS, EURAC, Deltares

Radio Astronomy
Univ. of Heidelberg, Max Planck Society

High Energy Physics
CERN, CNRS

Lattice QCD
CSIC, CNRS, ETHZ

Gravitational Wave - Astrophysics
INFN

https://www.intertwin.eu/use-cases/

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.

Interoperability & Link with DestinE

interTwin is conducting joint pilot activities with **DestinE** to **design a compatible architecture** that addresses the requirements of the largest set of user communities.

Interoperability is the aim of this activity.

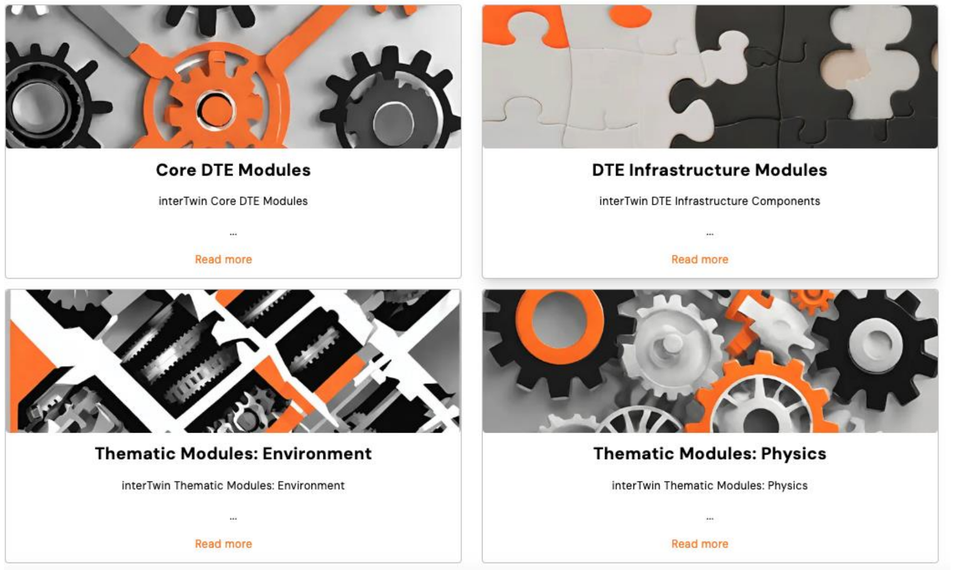
Demonstrators of data handling across interTwin and DestinE DTs for the Extremes and Climate in production-type configurations are under implmementaion in collaboration with **ECMWF**

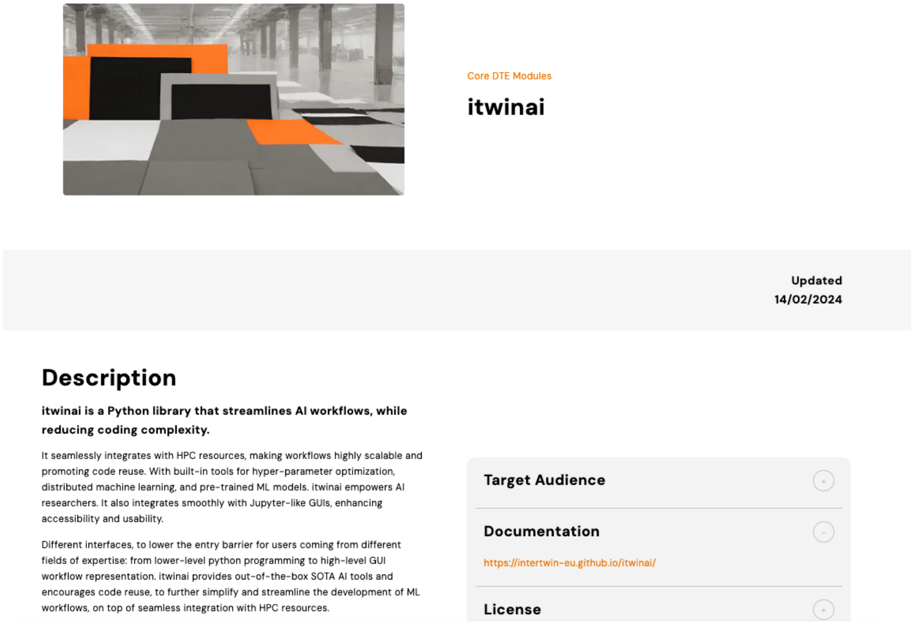
Part of the collaboration with DestinE includes the **development of common software architecture concepts** that are also **applicable to other major DTs initiatives**.

interTwin DTE First Release

interTwin DTE first release description available on our Website
https://www.intertwin.eu/intertwin-digital-twin-engine/

- 38 components in total
- New components developed and extension to existing software
- https://github.com/interTwin-eu





DTE Core components

Automated DT Validation in connection with workflow provenance

SQAaaS

yProv

Distributed data analysis embedded with specific workflow tools

Connecting Real-time data with serverless processing

Quality Verification

Workflow Composition

Big Data Analytics

AI / ML

Data fusion

Real-time data acquisition and processing

TOSCA Templates Repository

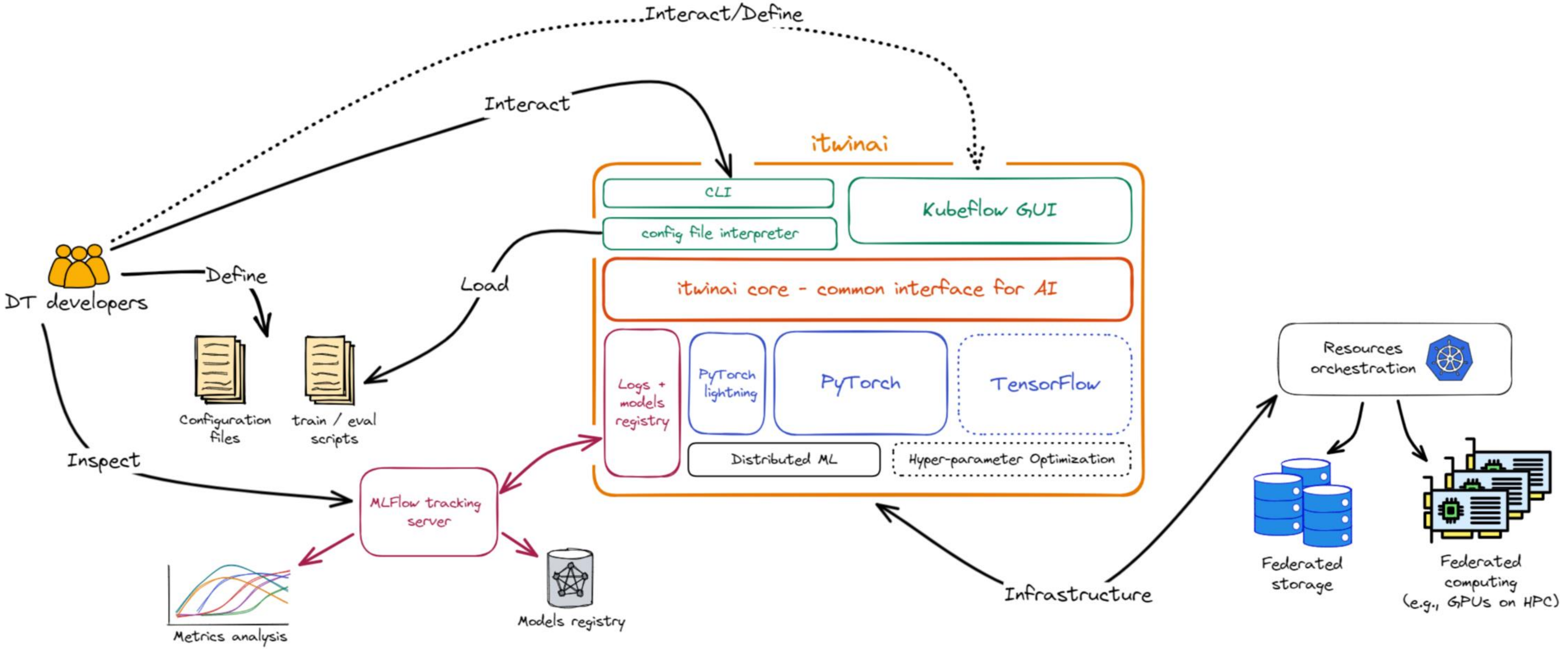
ANSIBLE Artifacts Repository

Standardized deployment of Big Data Analytics tools

itwinai

Generic ML / AI training platform with support to generic workflow management and model validation

itwinai - ML tooling for DT applications

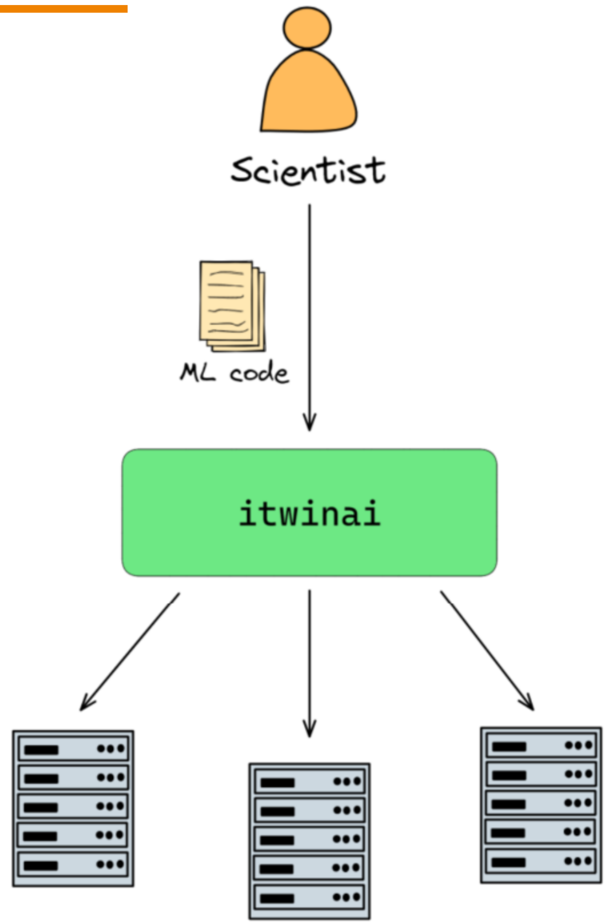


CERN contribution to the Core Engine

[Documentation](#)

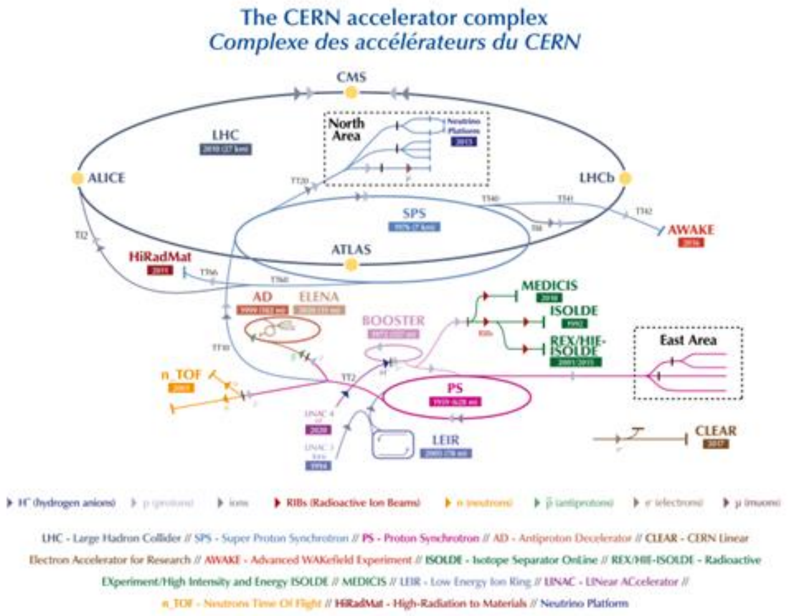
Support AI-based digital twin applications in science:

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



LHC & Particle Detectors in a nutshell

- Large Hadron Collider (LHC) is the world's largest and most powerful particle accelerator
- 27 km ring of superconducting magnets
- 2 high-energy particle beams travel at close to the speed of light in opposite directions, before they are made to collide
- beams inside LHC are made to collide at four locations around the accelerator ring -> positions of four experiments/particle detectors – ATLAS, CMS, ALICE and LHCb



(Images: CERN)

Detector simulation – WLCG Overview

- Simulation of particle transport through matter is fundamental for interpreting the results of HEP experiments
- Particles undergo complex interactions while traversing the detector material with stochastic outcomes

- These processes are modelled with Monte Carlo (MC) techniques that rely on repeated random sampling
- MC simulation meets the theoretical predictions with a high degree of precision but is time and resource intensive

- Worldwide LHC Grid has currently more than 50% of its resources focused only to simulation*
  - WLCG provides global computing resources for the storage, distribution and analysis of the data generated by the LHC
- Future High Luminosity LHC will require 100 times more simulated data**

* J. Albrecht et al., "A roadmap for HEP software and computing R&D for the 2020s," Comput. Softw. Big Sci., vol. 3, no. 1, p. 7, Mar. 2019
**G. Apollinari, I. A. BØjar, O. Brüning, P. Fessia, M. Lamont, L. Rossi, and L. Tavian, "High-luminosity large hadron collider (HL-LHC): Technical design report V. 0.1," CERN, Geneva, Switzerland, Tech. Rep. CERN-2017-007-M, 2017, pp. 1–516, vol. 4, DOI: https://doi.org/10.23731/CYRM-2017-004

WLCG
Worldwide LHC Computing Grid

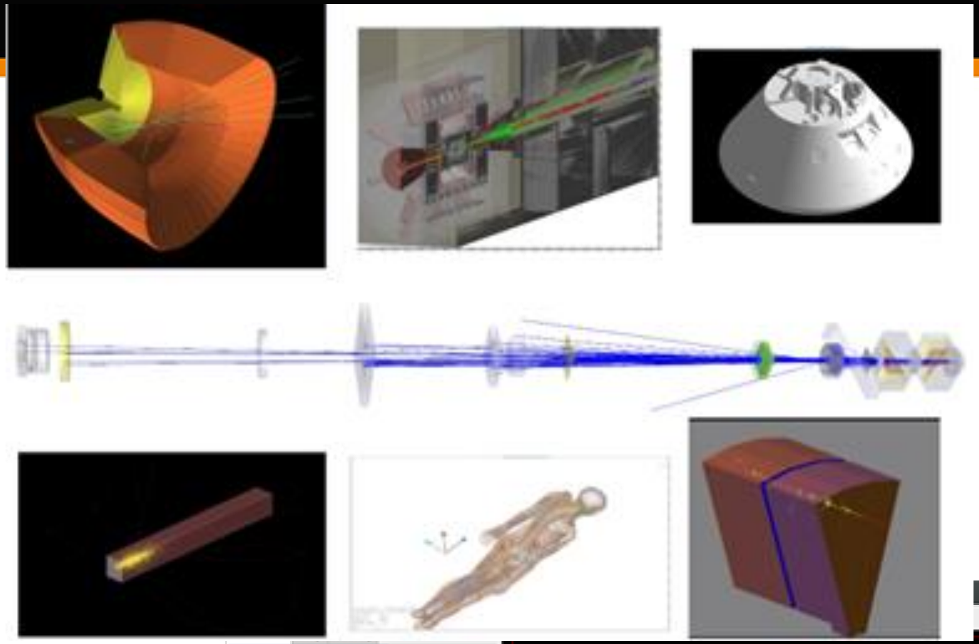
(Images: CERN)

Detector simulation – Geant4 overview

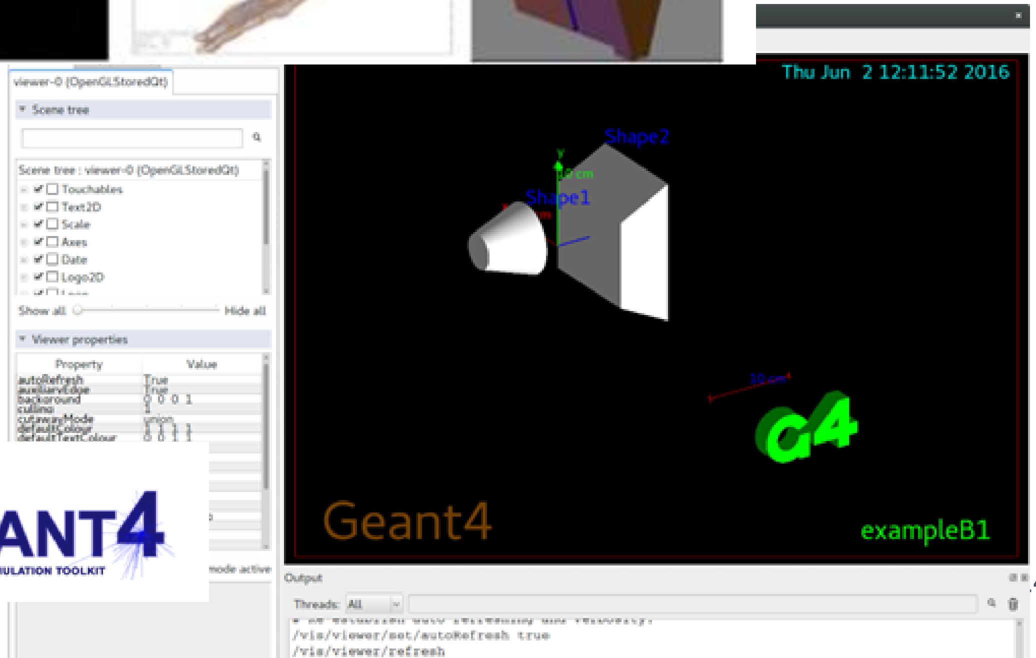
- Geant4 is an **open-source toolkit** that enables **simulating particle passage** through matter
- written in C++
- *toolkit* means that there is no main program provided
- provides all the necessary components needed to **describe and to solve** particle transport simulation problems in the form of **user interfaces**
- provides necessary **tools** for users to write their simulation applications

- **problem definitions/description:** geometry, particles, physics, etc.
- **problem solution**: step-by-step particle transport computation based on MC methods

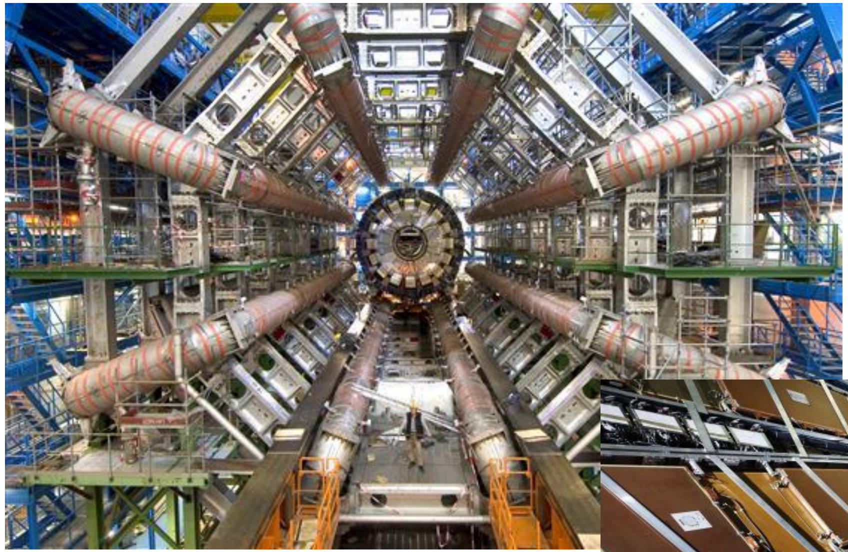
- each simulation problem requires different configuration that the user needs to define
- Visualization capabilities using OpenGL

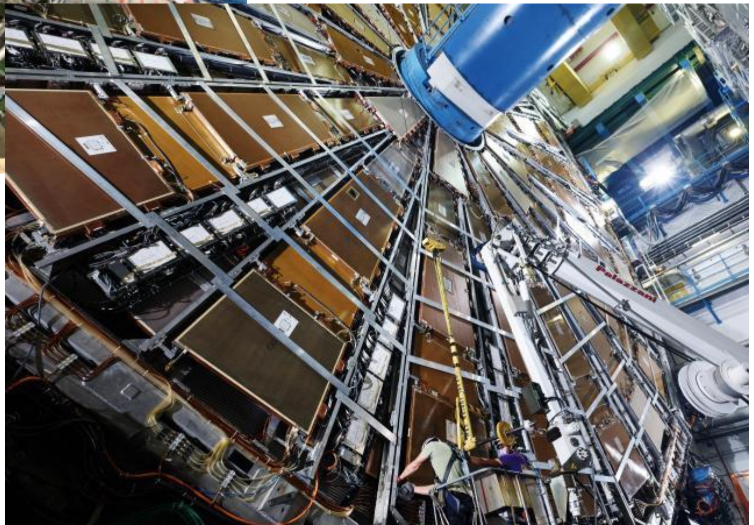


(Images: CERN)



Detector simulation DT - Motivation





The eight toroid magnets can be seen surrounding the calorimeter that is later moved into the middle of the detector. This calorimeter will measure the energies of particles produced when protons collide in the centre of the detector.

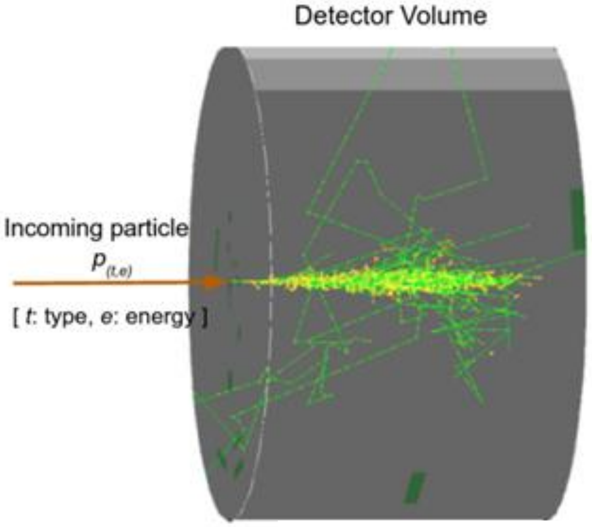
(Images: CERN)

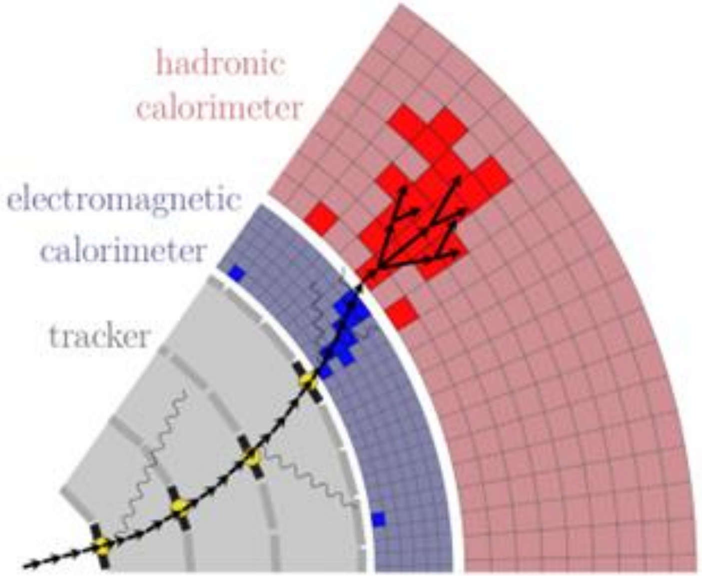
USE CASE CHALLENGES/MOTIVATION

- Particle detector simulations are fundamental for interpreting the results of HEP experiments, allow scientists to design detectors, and perform physics analyses

- Simulations are modelled with Monte Carlo (MC) techniques that rely on repeated random sampling:
    - inherently slow
    - complex multi-dimensional problem
    - substantial part of computing resources
    - calorimeters are the sub-detectors that are most time-consuming

Detector simulation DT - Solution



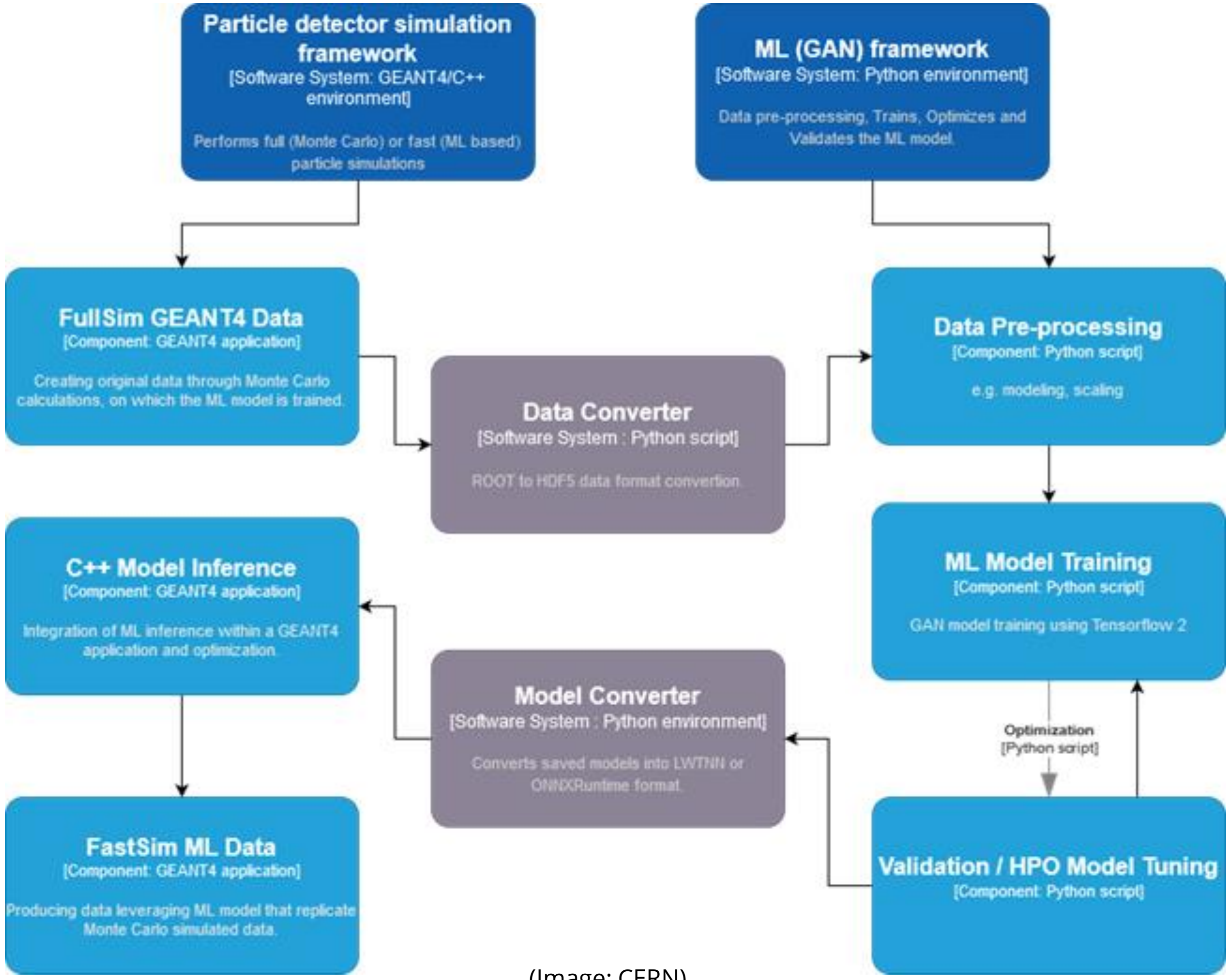


(Images: CERN)

SOLUTION

- HEP community highly motivated to explore *fast simulation*
- Fast simulation is a set of established techniques that replace parts of the detailed MC simulation with alternative approaches, including generative approaches (e.g. DL models), approaches based on parameterization and look-up tables, etc.
- We are leveraging a generative adversarial network approach developed at our lab, which has already shown promising performance as a standalone application so far.
- CERN's application will bring data-driven prototypes to production level by:
  - integrating Monte Carlo based solutions
  - establishing a flexible and detailed validation process

Detector simulation DT - Approach



(Image: CERN)

OUR APPROACH

- HEP detectors can be described as 3D cameras, taking high resolution pictures of particle collisions.
- Calorimeters detect particles by measuring the energy deposited in interactions with matter. They consist of arrays of active sensor material and passive dense layers, which ensure that the incoming (primary) particle will deposit most of its energy inside their volume.
- Energy depositions in calorimeter cells can be compared to the monochromatic pixel intensities of a 3D image.

Fast detector simulation DT - Activities

ACTIVITIES

- ✓ DT application design and capabilities, identified technical requirements
  - DT components:
    - simulation component that incorporates the Monte Carlo-based simulated datasets
    - deep learning component, which utilizes a generative model based on a specified particle detector set up

- ✓ Selected use case representing current challenges: Focus on calorimeters as detectors requiring the largest computing resources for simulation

- ✓ User stories that define the key functionalities and requirements (more in D4.2)

- ✓ First version of the DT capabilities (more in D4.4)

- ✓ Conducting research on more advanced generative models

Fast particle detector simulation with GAN

Goal:

- Optimising the Generative Adversarial Network (GAN)-based component developed for a selected set of detector geometries
- Integrating tools for distributed training and hyperparameter optimization.
- Implementing validation techniques capable of assessing different performance aspects

GEANT4: simulation toolkit that performs particle physics simulations based on Monte Carlo methods

- Faster alternatives to Monte Carlo, including DL-based techniques

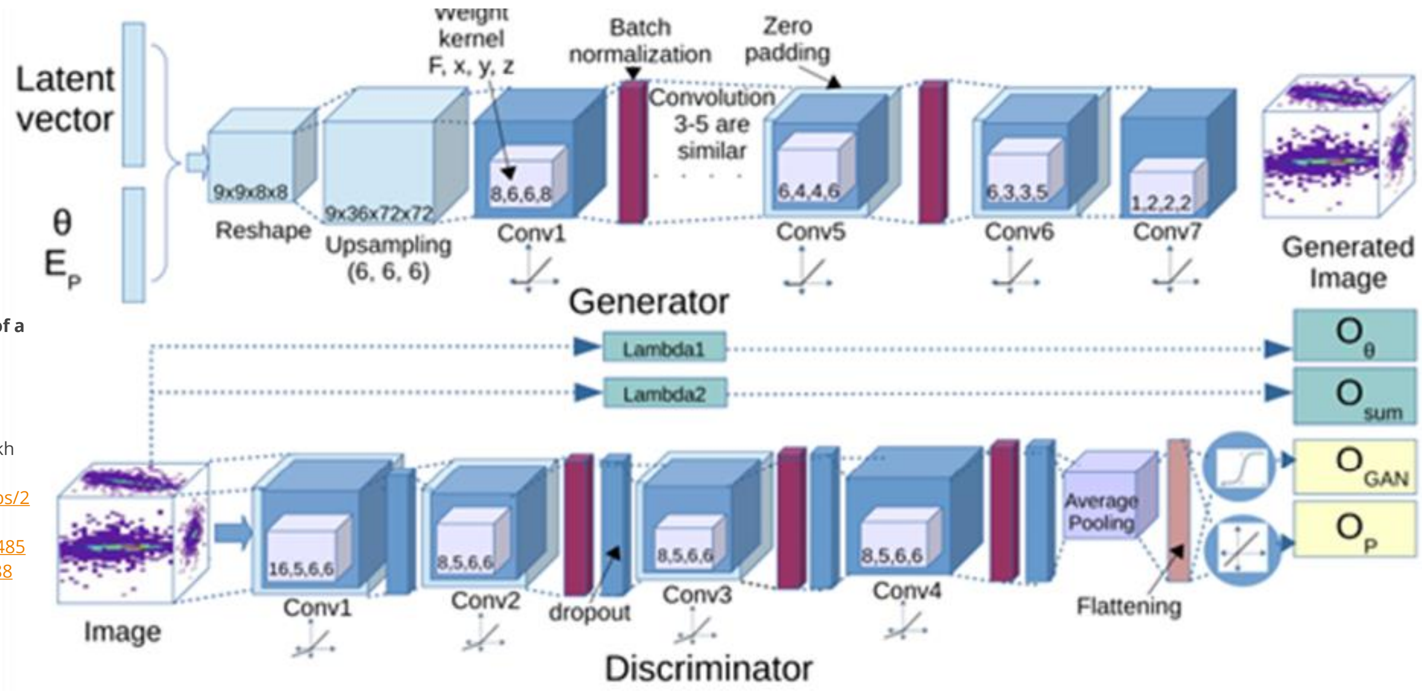
- Generative models: able to combine deep learning with statistical inference and probabilistic modelling
  - deep learning fast simulation generates directly the detector output
  - for the ML component of CERN’s thematic module, a Generative Adversarial Network (3DGAN) based model is being leveraged
  - three orders of magnitude speedup with respect to GEANT4

Fast detector simulation DT - 3DGAN

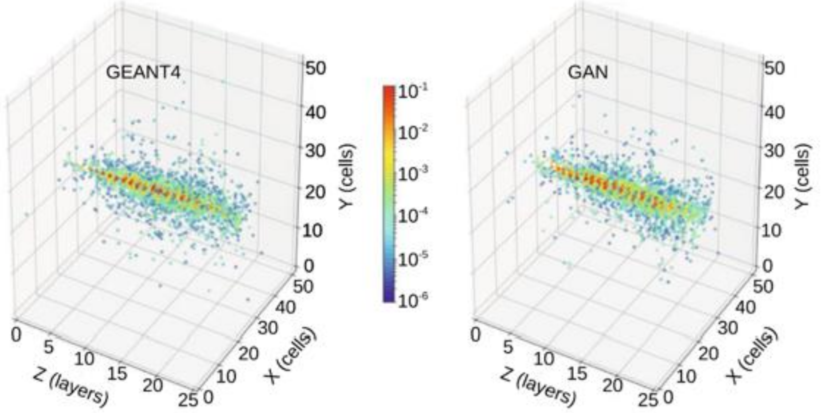
- For the ML component of CERN's DT, a Generative Adversarial Network based model is being leveraged
- 3DGAN: Simulation of a future high granularity calorimeter output as three dimensional images (51x51x25 pixels)*

- Three orders of magnitude speedup with respect to GEANT4

- Calorimeter cells are represented as monochromatic pixelated images with the cell energy depositions being the pixel intensities
- Our approach uses 3D convolution layers to represent the 3 spatial dimensions of the calorimeter image
- 3DGAN consists of 2 networks, the generator and discriminator



***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

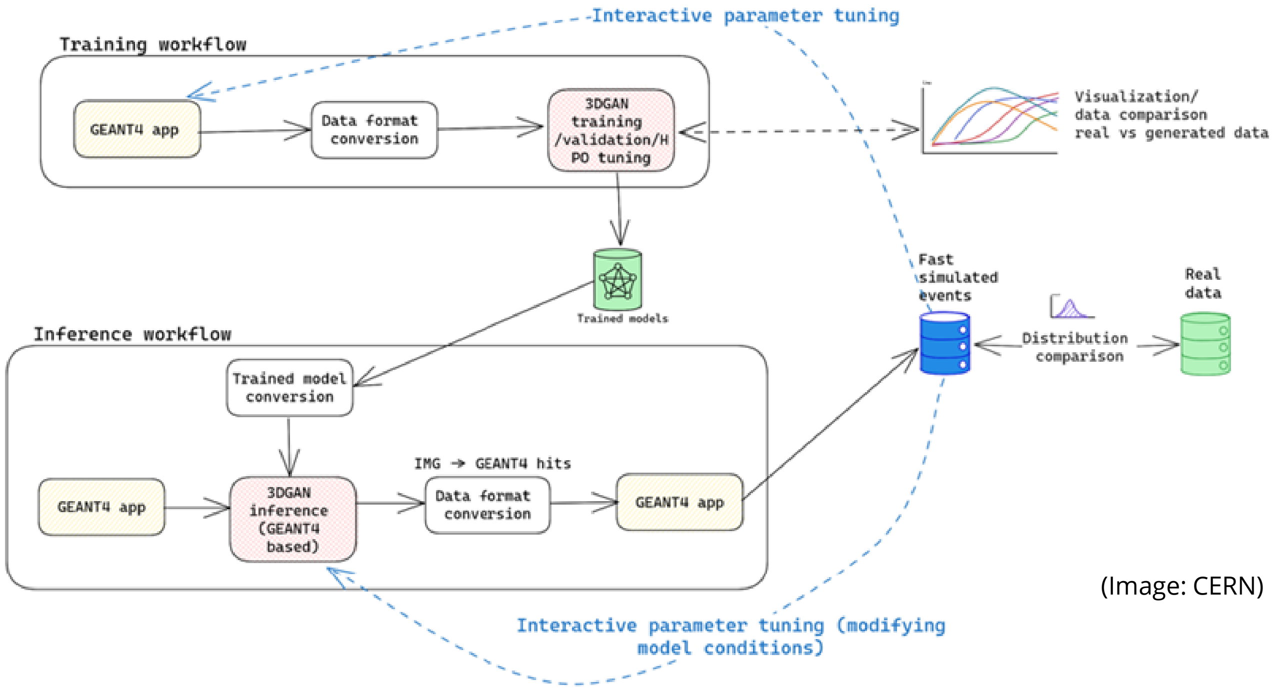


Example of a GEANT4 electron event (left) vs. an event generated by GAN (right) for the same initial conditions

(Images: CERN)

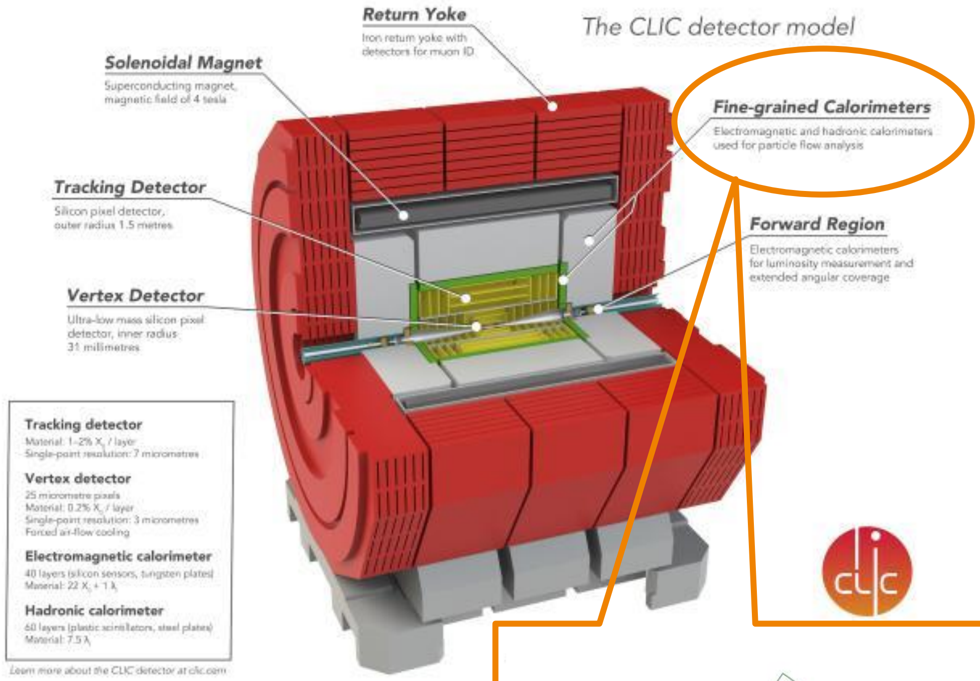
Fast detector DT training and inference workflows

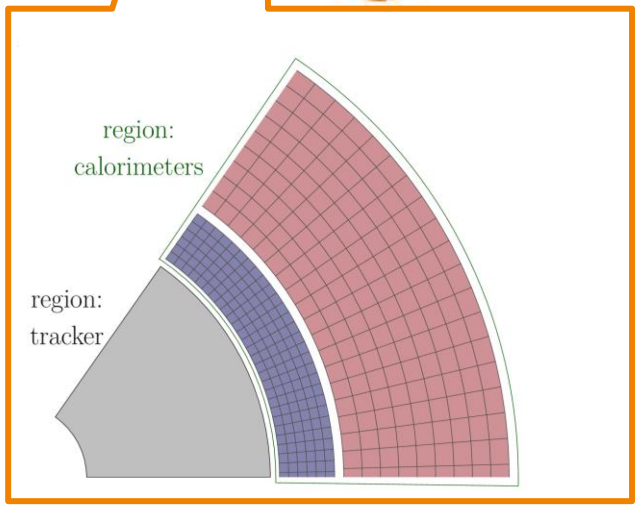
- **Generate input data for training**
  - Run Monte Carlo simulations locally using GEANT4 software → Output: ROOT files
- **Pre-process ROOT files before feeding the data into the ML model**
  - Input: ROOT files → Output: HDF5 files (decreased volume)
- **Store input and output data**
  - Object or local storage
- **Distributed training with multiple GPUs**
  - GANs, to be tested: Transformer-based models
- **Model inference**
- **Validation/Quality Check**
  - Comparing generated data with Monte Carlo data
  - Sample-based metrics
- **Continuous re-training**
  - Current state of use case (as described in proposal) is a static synthetic model of a detector.
  - Exploring of extending to an application capable of modelling in real time the detector's output in different operation conditions (beams and accelerator configurations) → continuous re-training on real data



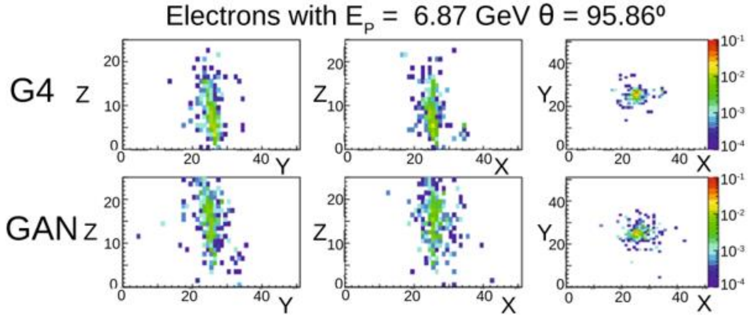
(Image: CERN)

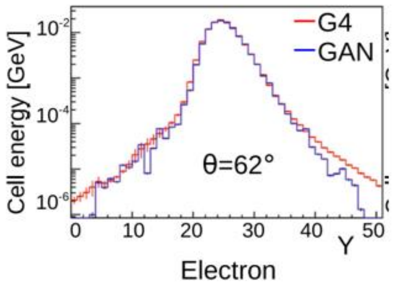
Fast detector simulation DT - 3DGAN (2)

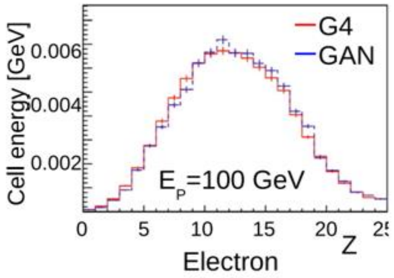


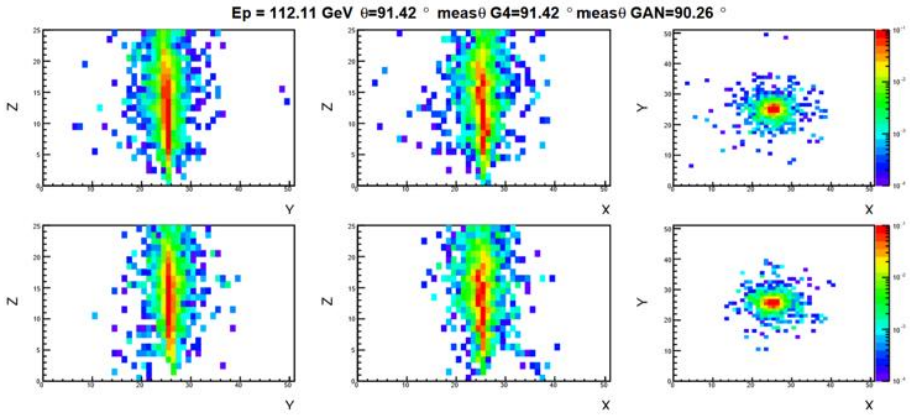


Images: CERN & **Fast Simulation of a High Granularity Calorimeter by Generative Adversarial Networks.** Gul Rukh Khattak et al. https://arxiv.org/abs/2109.07388
DOI: https://doi.org/10.48550/arXiv.2109.07388









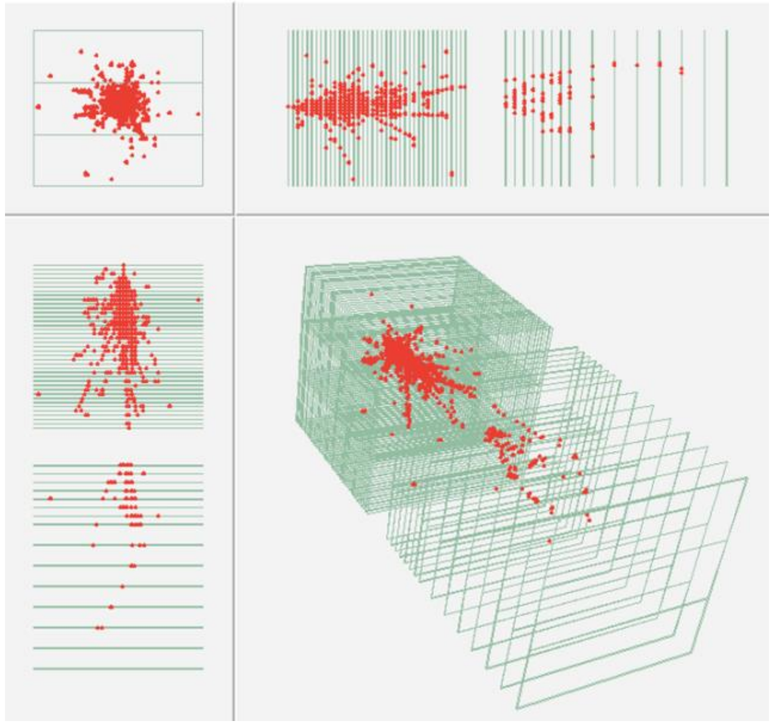
DT integration activities w/ DTE core modules

We've developed a DT of the calorimeter detector of the CLIC CERN particle detector

- first release will include the 3DGAN component which is trained on data coming from simulations run with Geant4 within an application set up of the selected detector's geometry

The first phase of the Particle Detector Simulation DT, which includes the 3DGAN component has been integrated with:

- AI workflows framework: itwinai
- Workflow execution: OSCAR
- Federated computing: InterLink
- Quality assessment: SQAaaS



W-DHCAL event display (Image: CERN)

For even more detailed description on the integration activities please see the demo curated by our colleagues and also navigating in itwinai documentation page!

Fast particle detector DT - Future plans

FUTURE PLANS:

- Exploring integration to MC-based framework and optimization of the data transformation pipelines.
  - Integration of the GAN models with the MC-based framework (GEANT4) will be implemented.

- Develop or integrate tools for parallel training and hyper parameter optimization (modified to accommodate the adversarial training process, if needed).
  - Focus on solutions best adapted to the specific GAN use case, considering the specific features of the available computing hardware (in terms of accelerators and internode communication)

- Customizable validation framework will be developed in collaboration with HEP community experts.
  - implementation of complex multivariate distributions based on a large range of input conditions
  - validation techniques capable of assessing different aspects of performance, including accuracy and comparison to classical Monte Carlo, i.e. uncertainty estimation, coverage of the support space

- Further development of the DT's thematic modules

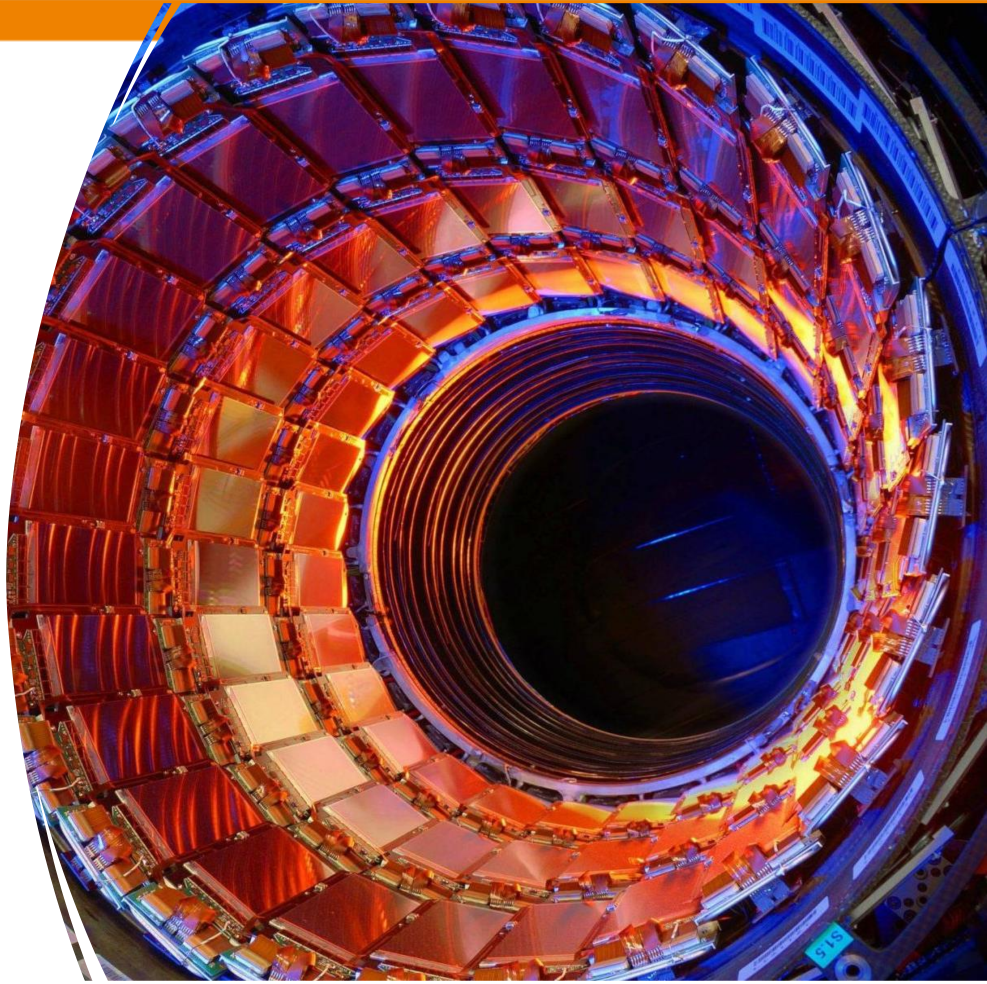
- Integration and test compliance of our software components with the DTE core modules

THANK YOU!

QUESTIONS?

Contact details:

- Kalliopi Tsolaki: kalliopi.tsolaki@cern.ch
- Matteo Bunino: matteo.bunino@cern.ch
- Sofia Vallecorsa: sofia.vallecorsa@cern.ch



Annex

- interTwin: https://www.intertwin.eu/

- References:

[1] Khattak, G.R., Vallecorsa, S., Carminati, F. et al. Fast simulation of a high granularity calorimeter by generative adversarial networks. Eur. Phys. J. C 82, 386 (2022). https://doi.org/10.1140/epjc/s10052-022-10258-4

[2] J. Albrecht et al., “A roadmap for HEP software and computing R&D for the 2020s,” Comput. Softw. Big Sci., vol. 3, no. 1, p. 7, Mar. 2019

[3] G. Apollinari, I. A. BØjar, O. Brüning, P. Fessia, M. Lamont, L. Rossi, and L. Tavian, “High-luminosity large hadron collider (HL-LHC): Technical design report V. 0.1,” CERN, Geneva, Switzerland, Tech. Rep. CERN-2017-007-M, 2017, pp. 1–516, vol. 4, DOI: https://doi.org/10.23731/CYRM-2017-004

[4] https://g4fastsim.web.cern.ch/