Scientific Computing & Digital Twins

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CSIC
Consejo Superior de Investigaciones Científicas
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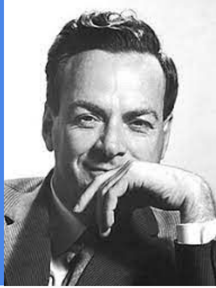
Background

- Physics is an experimental science: we investigate where we can
- Usually following the so-called "*Streetlight logic*":

  "if you walk back home in the night, and have lost your keys, look for them in the illuminated area, because you will not find them anywhere else"

- History shows that Science advances like that: sometimes unexpected things are found, more interesting than the expected ones

How does one formulate a new Physics law?



1. First, we guess it
2. Second, we compute the consequences of that guess
3. Third, we compare with Nature: i.e. with experimental observations

We informed Richard Feynman that his role would be to advise on the application of parallel processing to scientific problems. "That sounds like a bunch of baloney," he said. "Give me something real to do."

(Daniel Hillis, in "*Richard Feynman and The Connection Machine*")

Background

How does one formulate a new Physics law?

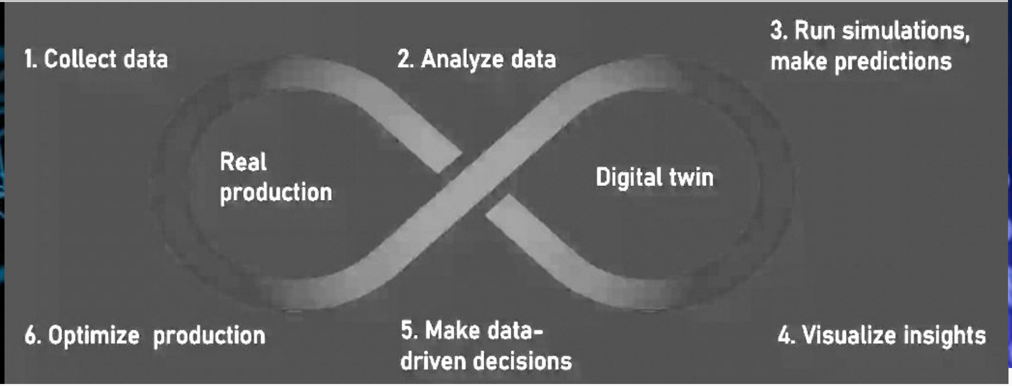
1. **First, we guess it**
2. **Second, we compute the consequences of that guess in measurable terms**
3. **Third, we compare with nature: i.e. compare with experimental observations**

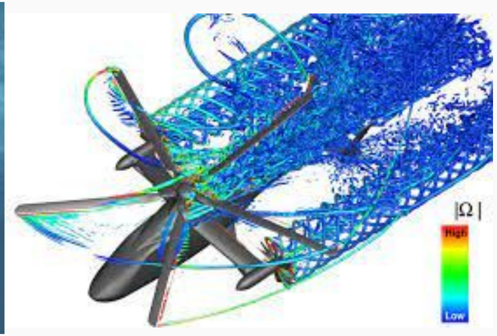
- Our “core business” as community is advancing computing technologies to support scientific challenges.
- Looking for solutions for specific Scientific & Technological challenges notably for steps (2) and (3)
- Some are even trying to apply Artificial Intelligence to (1). The value of knowledge without understanding is however very limited.

We are trying to exploit the technologies associated with Digital Twins (an industrial concept born in aeronautics) to improve research capabilities in HEP, Observational Astrophysics, Extreme phenomena, Geophysics, Climate predictions, etc…

How are “our simulations” related to the concept of Digital Twins

When does a Simulation become a Digital Twin ?





Background

How did it all began ? Simulator of the Apollo 13 mission at NASA

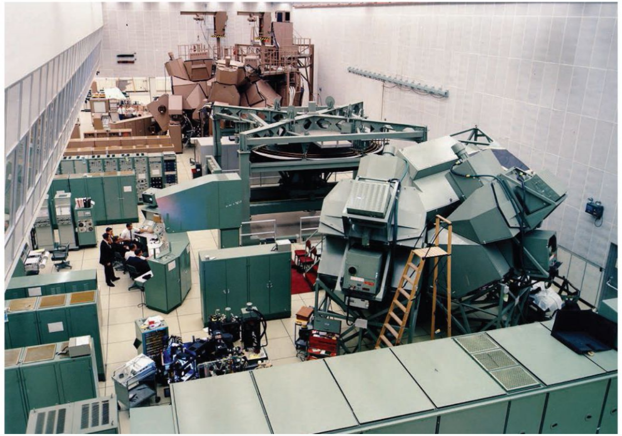
The idea of a “digital twin” was born at NASA in the 1960s as a “living model” of the Apollo mission.

→ In response to Apollo 13’s oxygen tank explosion and subsequent damage to the main engine

→ NASA employed simulators to evaluate the failure and extended a physical model of the vehicle to include digital components.

→ This “digital twin” was the first of its kind, and was able to rescue the mission by simulating

Apollo Simulators installed at NASA - Front - Lunar Module Simulator (green)
Mid- Mission Effects Projector-Lunar surface (green)
Back - Command Module Simulator (tan)

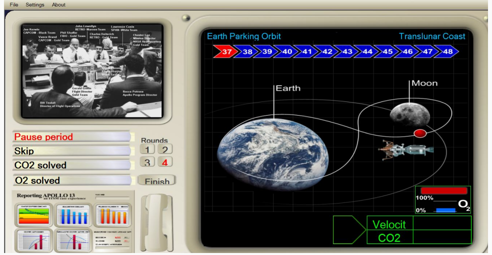


“Keep ‘em Running,” screamed Astronaut Eugene A. Cernan as he strode into the simulator room late on that fateful Monday night.”

(Connecting Link magazine, Summer 1970 issue)

“The countless improvisations that nursed the crippled spacecraft along were in large measure the product of an extraordinarily elaborate assembly of simulators at the Manned Spacecraft Center in Houston and elsewhere. Every makeshift procedure carried out in space was first tried out on earth, and rejected if the simulators showed it to be dangerous or impractical.”

(New York Times, on the Apollo 13 accident)



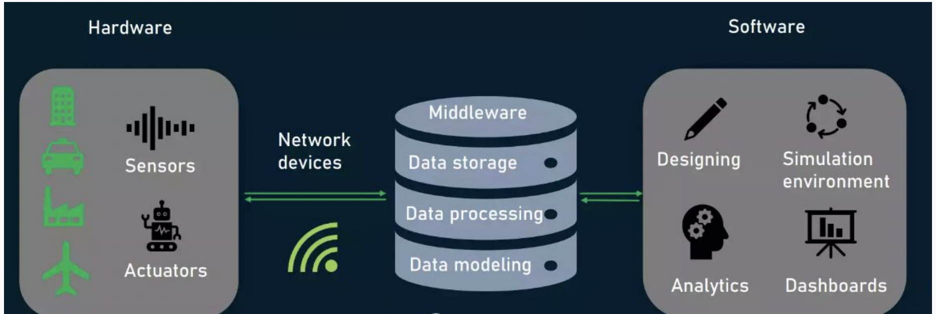
Elements of a Digital Twin

Hardware components. Measuring devices, sensors, etc… that initiate the exchange of information between reality and their software representation.

Data management middleware.A repository to accumulate data from different sources. Ideally, also takes care of data integration, processing, data quality control, etc… by interacting with software components

Software components.

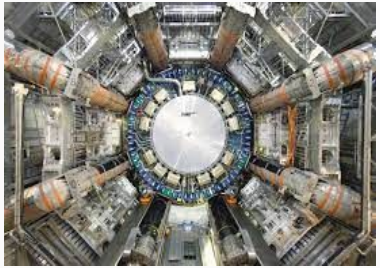
- The analytics engine that turns raw observations into predictions by the simulation software
- In many cases, powered by machine learning models.
- Other: dashboards for real-time monitoring, design tools for modeling etc…

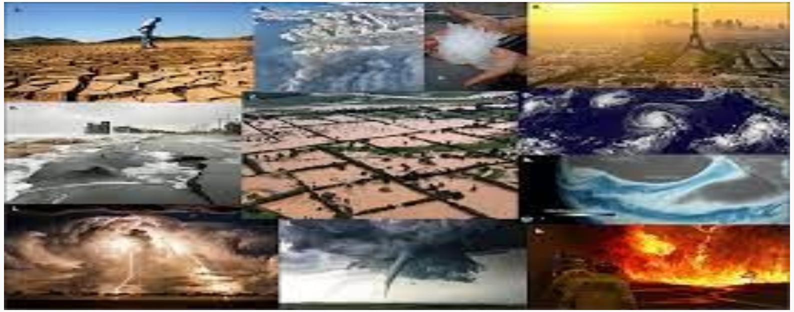


interTwin

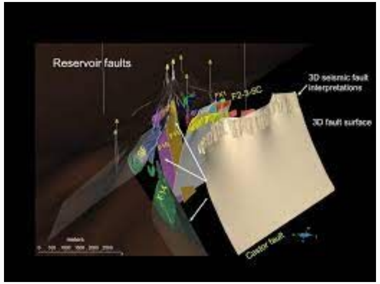
DT-GEO

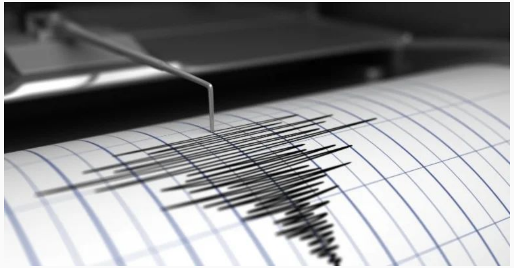
InterTwin → Interdisciplinary





DT-GEO → Geophysical extremes





Digital Twins in HEP and Astro

→ Fast Algorithms for Detector Design based on GANs

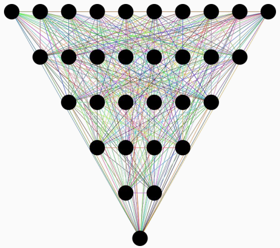
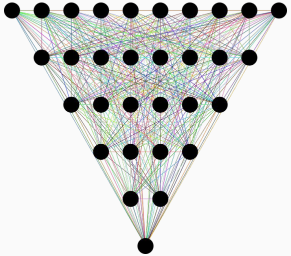
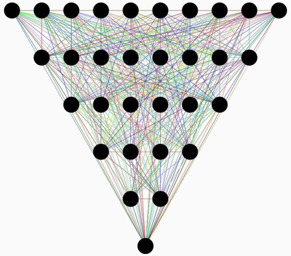
→ Theoretical Computations and Simulations

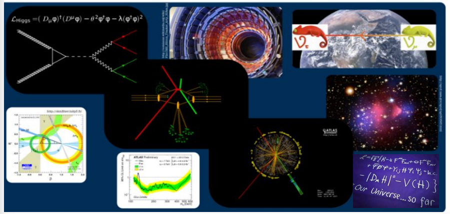
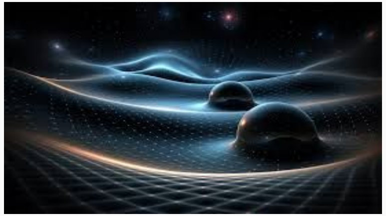
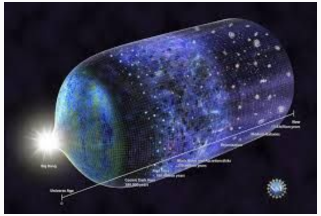
Machine Learning tools to accelerate the simulation with respect to conventional Monte Carlo

Machine learning to help detecting noise in signals

interTwin



Elementary Particles

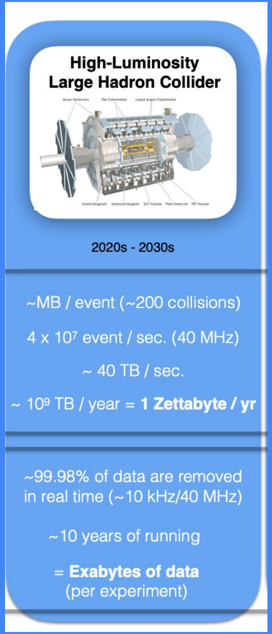
Gravitational Waves

Dark Matter

Digital Twin def.

A digital twin is a **digital model of an intended or actual real-world physical product,** system, or process (the physical twin) that serves as digital counterpart for practical purposes:

- simulation,
- Integration with other systems
- Testing with real data,
- Monitoring behaviour,
- maintenance,...



In HEP we search for ever smaller signals in ever larger data sets

- It applies to both data analysis and simulations
- Large streams of data from observational facilities
- Large data ensembles coming from simulations
- Data detectors subject to many sources of noise
- Real-time online analysis capabilities

The distinction between Online and Offline requirements becomes fundamental

Digital Twin	Reality and Simulation challenge
LHC detector ~ Apollo 13	**Reproducing the response of the detector when hit by highly energetic particles ~ response of Apollo 13 to the operation conditions in space**

Machine Learning in Particle Physics requires the understanding of the opportunities to deploy ML methods Online and Offline

- Multivariate analysis is commonplace in HEP data analysis since the 1990's
  - **TMVA** software package has been the standard
- There is a more diverse ecosystem: many people relies now on industry standards such as SciPy TensorFlow and PyTorch

Industry drives Machine Learning but Science in general requires dedicated solutions

- The level of precision required for **data-simulation hybrid methods** calls for **specific research in uncertainty quantification and validation**
- Explore **physics-aware learning** with custom ML architectures
- **Generative models** accelerate various steps in the simulation chain: eg. in HEP in relation to Physics generators, detector simulation and lattice gauge theory.

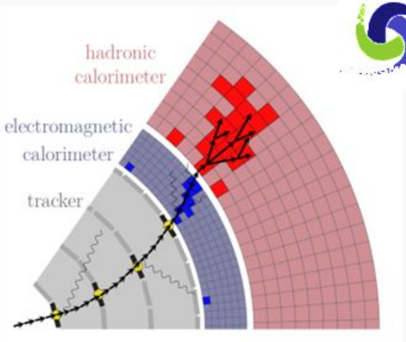
High Energy Physics: DT of a HEP detector

Detector Simulation Software = Software that simulates the physics processes happening at the detector level
GEANT4 is the golden standard software for detector simulations:

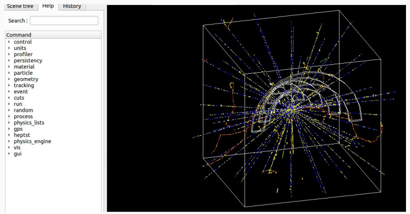
→ **Passage of particles through matter, in particular through the materials a particle detector is made of. Expensive to run (40% of the time spent in all the MC simulations needed)**

→ Machine learning (ML) provides a complementary approach: by **learning a map between incident particles and detector response using GEANT4 as reference result.**

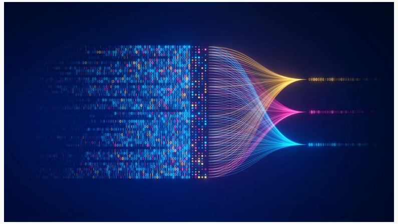
Using ML to accelerate detector simulation is a popular option currently under investigation

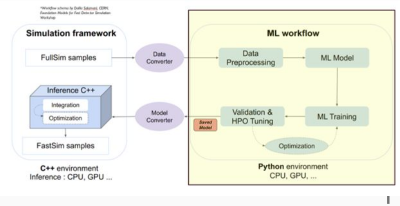


GEANT4
A SIMULATION TOOLKIT



See Alexander & Matteo´s presentation today





A multi-layered "reality": This DT implies taking as "reality" a MC simulation

- The physics processes need to be simulated as well: physics models are programmed in GEANT4 (458 pgs. Physics Reference manual)

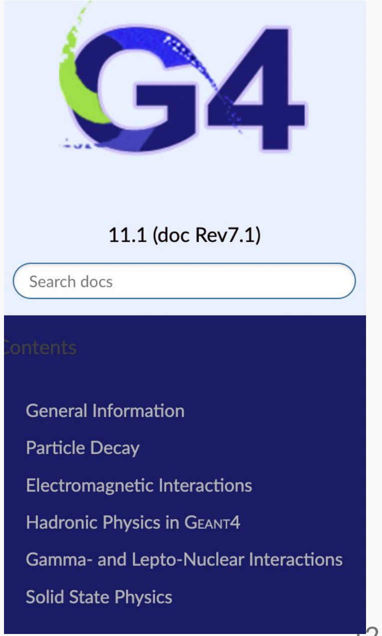
  Change the physics models/parameters simulated

  —> changes the response of the DT

  There are model-related uncertainties ? How do we deal with it ?

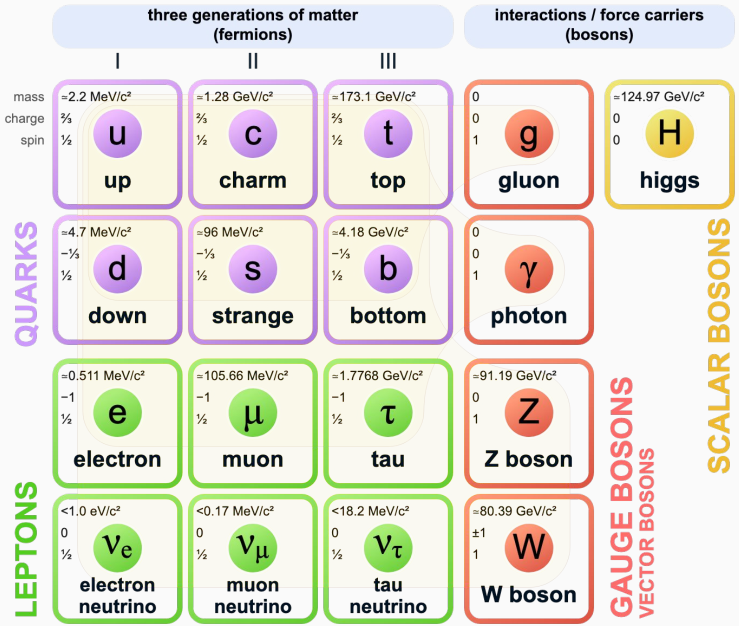
- Future detectors are highly complex, many different parts and materials involved: Full detector simulation is a very long term goal:

  Current fast ML simulation techniques require using hundreds of separately trained models to describe the response of each detector element, to each type of physics process.

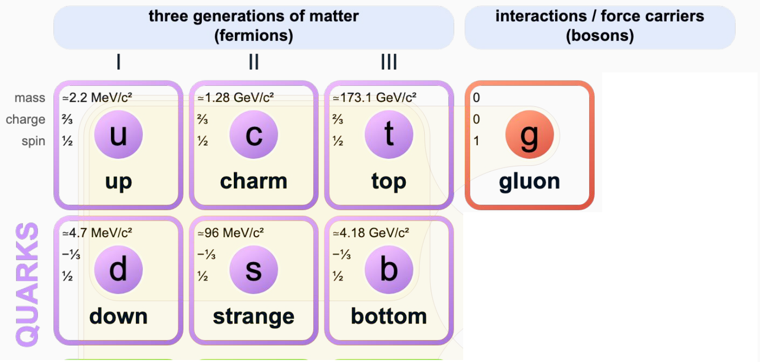


High Energy Physics: the quest for reality

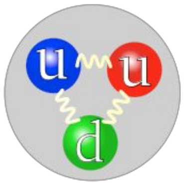
Standard Model



Quantum Chromo Dynamics part

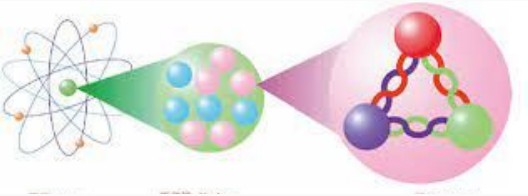


Strong force



High Energy Physics: Lattice QCD
“First, we guess it”

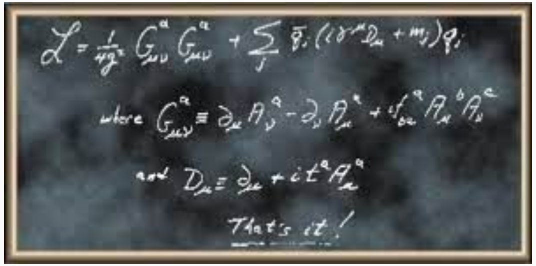
“Reality of interest”: Quantum Chromo Dynamics



QCD is believed to explain why quarks are confined inside hadrons

Real data: from particle accelerators experiments

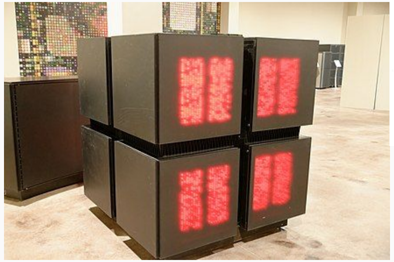
Matching with simulations is the subject of an entire subarea of HEP : Phenomenology.



Is Lattice QCD actually a Digital Twin of the underlying particle physics real world ?
The question is different, because we do not really know how the real world looks like

High Energy Physics: LQCD > 30 years of development

Second, we compute the consequences of that guess



1985 - Connection Machine

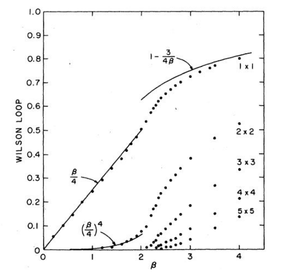
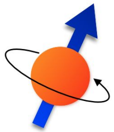


FIG. 4. Wilson loops as a function of β.

← **From the toy model, to**

probing the Standard Model →

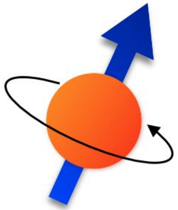


g-2 = 0.00233184110
+/- 0.00000000043 (stat.)
+/- 0.00000000019 (syst.)

"Feynman had to write a computer program to test the machine. Since he only knew BASIC, invented a parallel version of BASIC, and programmed QCD. He was excited by the results. ***"Hey Danny, you're not going to believe this, but that machine of yours can actually do something useful ! "*** *(Daniel Hillis, in "Richard Feynman and the Connection Machine")*

The anomalous magnetic moment of the muon: g-2

What is a muon?



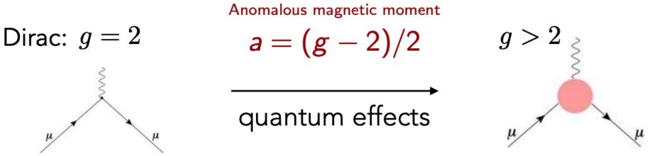
- Elementary point-like particle
- Same electric charge as an electron
- Approximately **200** times heavier than an electron
- Like the electron, behaves as if it was intrinsically spinning about a vector $\vec{S}$

These properties combine to give it a magnetic moment

$$\vec{\mu} = g\left(\frac{e}{2m}\right)\vec{S}$$

such that when put in a magnetic field, it exhibits precession similar to a spinning top.

We can measure this precession **very** precisely.



The quantum effects arise from virtual particle contributions from all known **and unknown** particles.

"First results from the Muon g-2 Experiment at Fermilab"
https://indico.cern.ch/event/1019685/

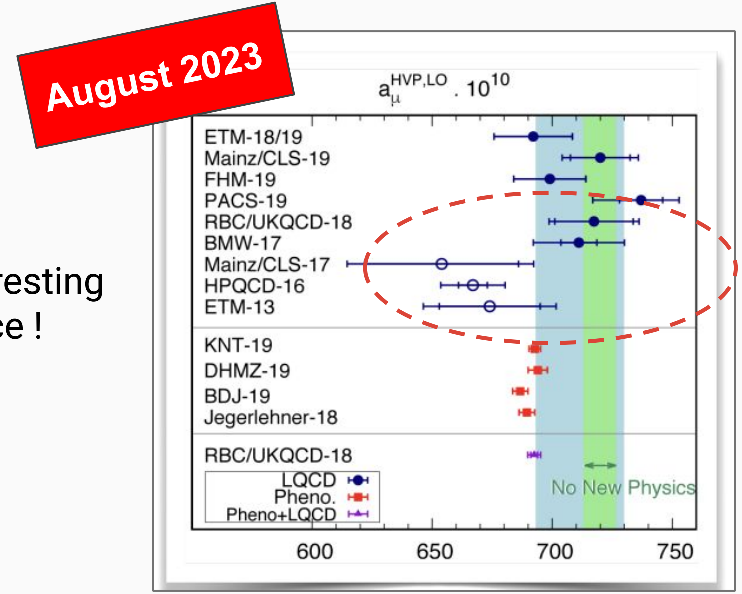
High Energy Physics: Lattice QCD - towards the Exascale Computing era

We gather data to measure (g-2):

A. In experimental facilities: the answer of nature. Several experiments ongoing
B. In the HPC systems by simulating the Standard Model (the QCD part)

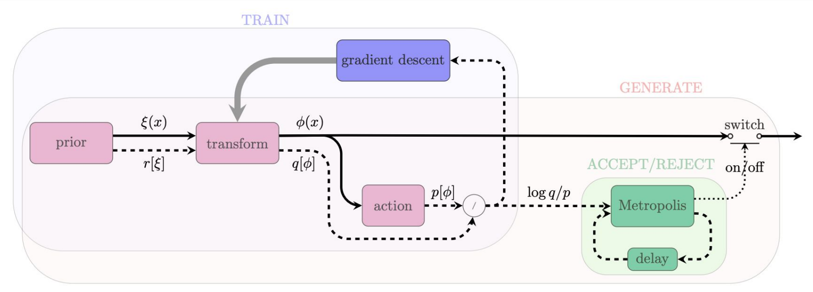
if (A) is compatible with (B) the Standard Model stands correct

Interesting race !



Machine Learning in Lattice QCD

- Speeding up the generation of QCD configurations in complex areas of the parameter space.
- The Machine Learning process learns on the results of the full Monte Carlo simulation, comparing the results of reference observables (eg. energy) with those obtained using reference codes (eg. OpenQCD).
- Designing better architectures for Machine Learning models so that the acceptance rates become reasonable (~50% or more) as the volume of the lattice increases.



VIRGO experiment

Measuring the disturbance of space-time following a galactic “cataclysm” (eg. black holes colliding, neutron stars collisions, etc…)

Digital Twin of the Interferometer

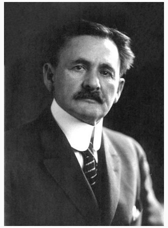
→ To realistically simulate the noise in the detector, in order to study how it reacts to external disturbances

→ To be able to detect noise in quasi-real time to inform the online pipelines, which is currently not possible.

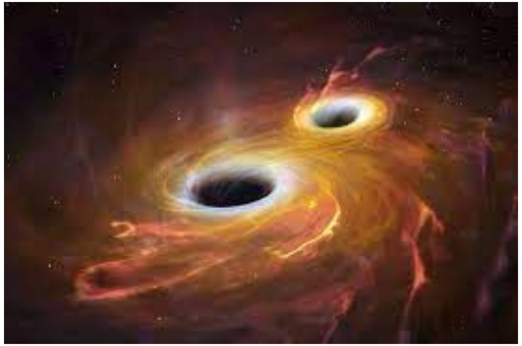
Following true cosmic cataclysm
eg. collision of two black holes

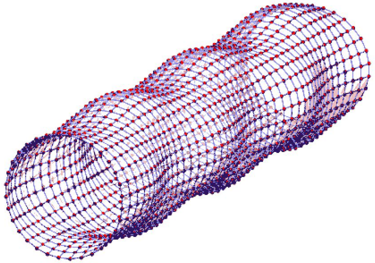
Gravitational Waves are generated:
extremely non-intuitive but true →

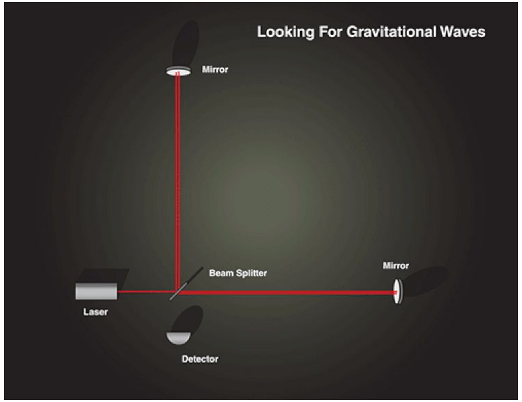
The detection of the distortion of space-time is a challenging experiment here on Earth



1907 Nobel Prize,
Albert Michelson





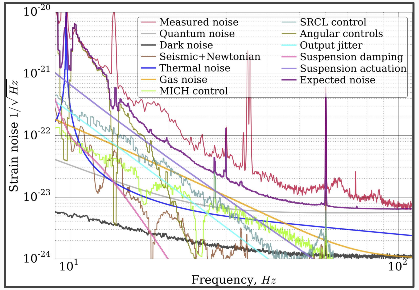


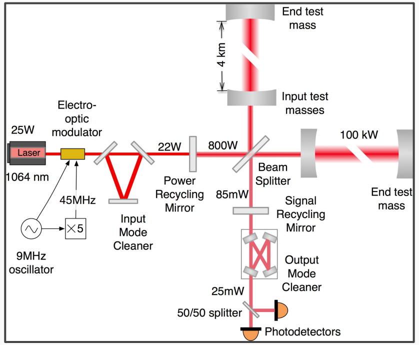
Digital Twin of a 3km long-arms Michelson interferometer

The experiment needs to measure a very faint signal

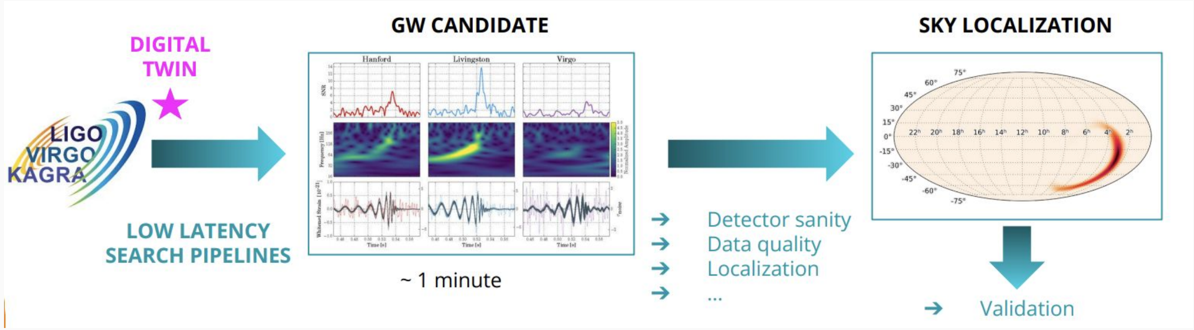
Removing the noise in the experiment is key:

A proper simulation of that noise is crucial to increase the sensitivity of the detectors

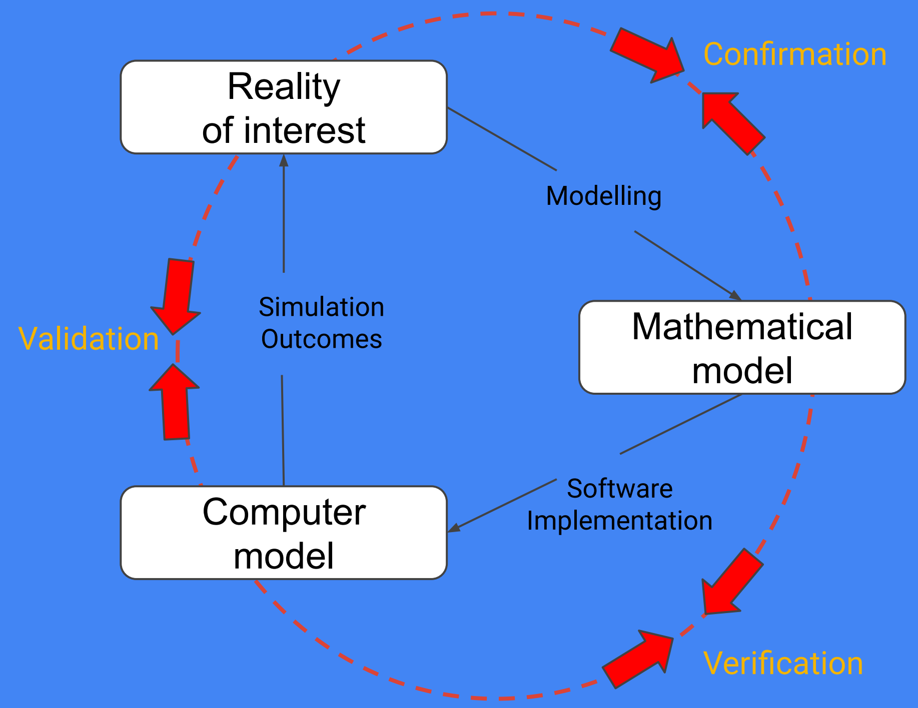




- **Seismic noise**, movements earth vibrations
- **Thermal noise**, from the microscopic fluctuations of the individual atoms in the mirrors and their suspensions.
- **Quantum noise**, due to the discrete nature of light
- **Gas noise**, from the interactions of the residual gas particles in the vacuum enclosure with the mirrors and the laser light.
- **Laser noises**, small variations in the laser intensity and frequency.
- **Beam jitter**, or slight variations in the position and angle of the laser beam in the detector,
- **Scattered light**, generated by tiny imperfections in the mirrors of the interferometers
- And finally, **electronics noise**



Verification, Validation & Uncertainty Quantification



At what point does a simulation becomes a Digital Twin?

Quoting old NASA minutes

*"What matters is the **significance of the effect that you are trying to model w.r.t. to variables that you are interested in**. An animation of variables on the surface there doesn't make the system a DT because it lacks fidelity for the purposes of the operations.*

*Is there a fidelity "slider" from sim to DT? Ask whether its meaningful to what you're predicating. It's a question of uncertainty and validation. Is it good enough to drive operations? **A simulator (like LITE) never changes**.*

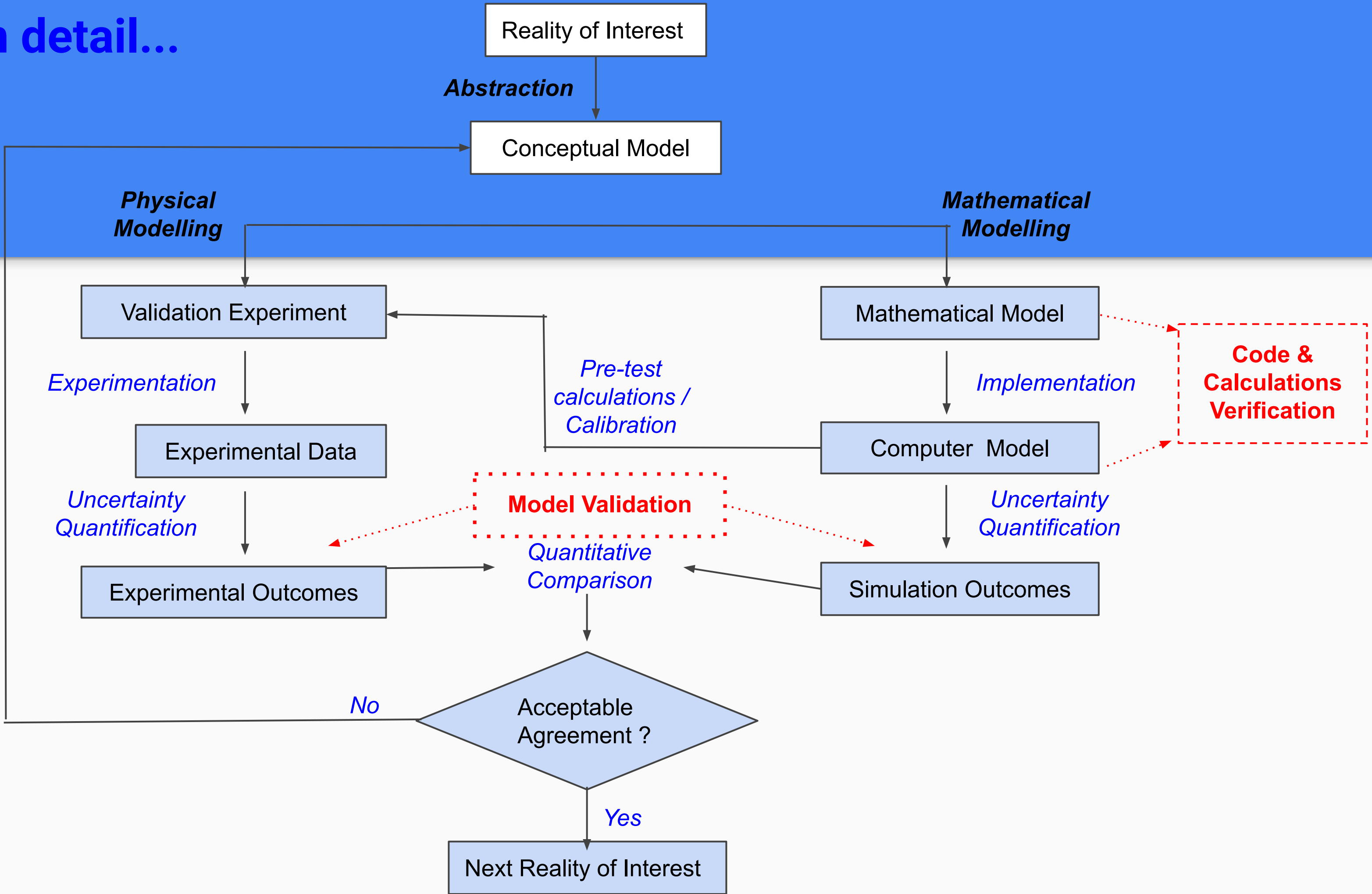
*DT changes over time. • **DT changing over time** = persistent simulation over life of asset or system. **Co-evolution of digital artifact with physical artifact***

*• Conclusion: **identification of validation criteria for then is your DT good enough of a twin?** Gravity variable is potentially a game changer. Lack of air (vacuum). **Need serious thinking about what validation is"***

Take outs

- A simulation is not a Digital Twin unless you can prove it corresponds to the evolution of reality as well
- Validation is the process to prove it
- Comparison and feeding input with real data is key

More in detail...



Better Climate models to understand how the climate evolves

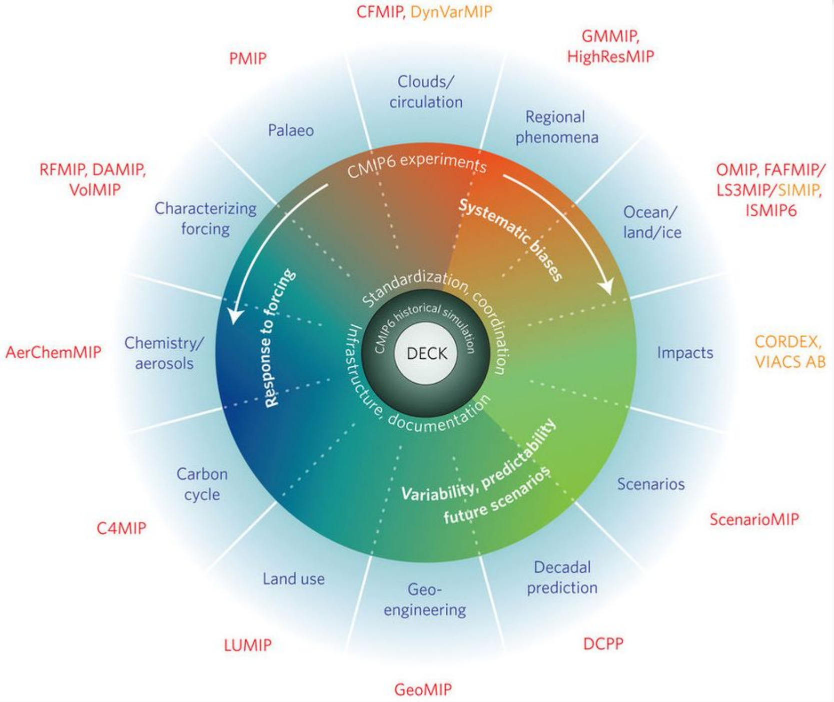
Example: Program for Climate Model Diagnosis and Intercomparison

- Those models simulate the physics, chemistry and biology of the atmosphere, land and oceans.

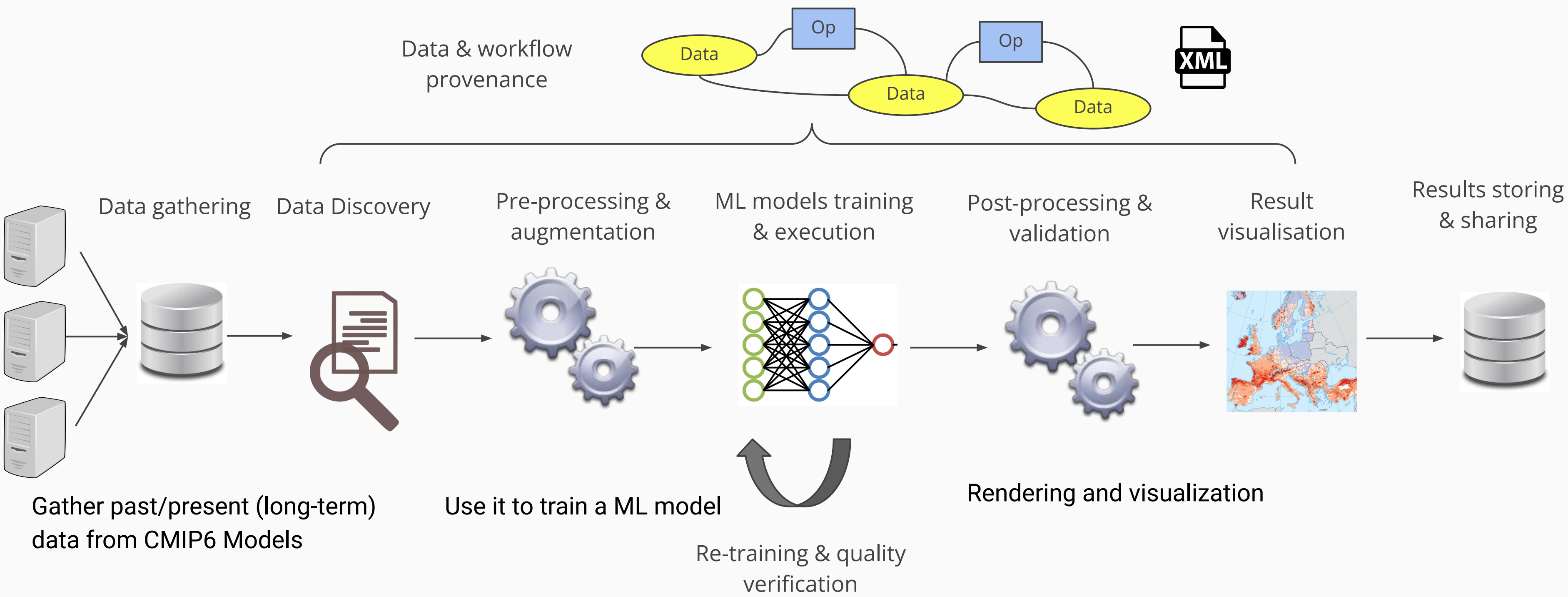
- Climate models are constantly being updated: incorporating higher spatial resolution, new physical processes and bio-geo-chemical cycles.

- The results of the simulations are updated in coordination with the IPCC reports. These efforts are coordinated by the Coupled Model Intercomparison Projects (CMIP) WG.

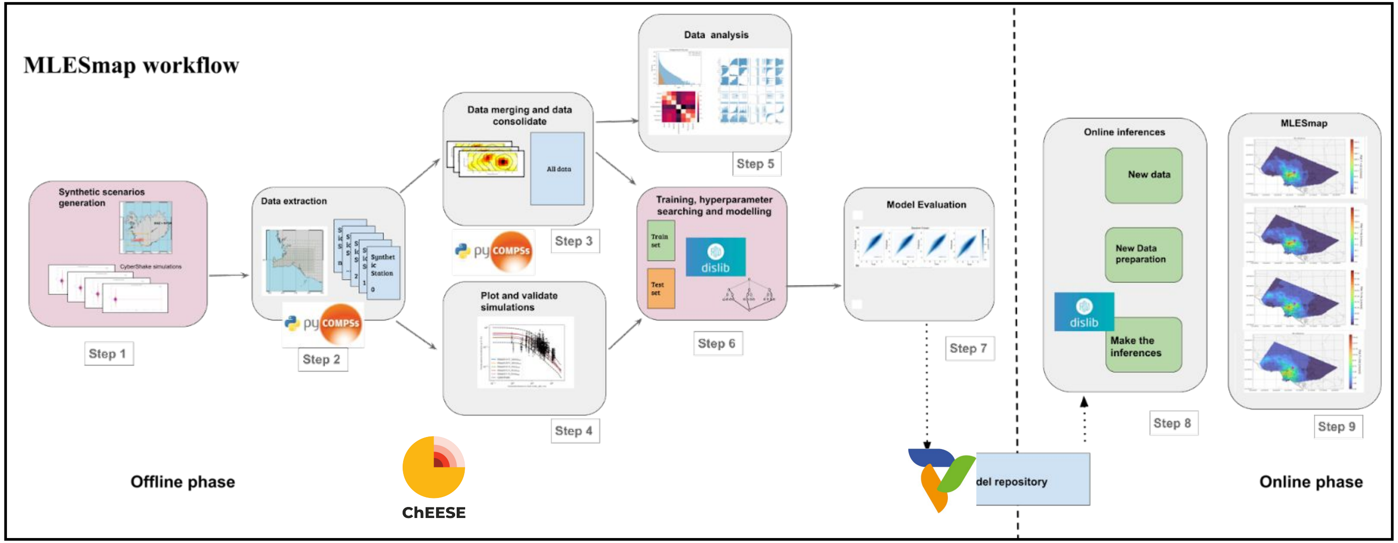
- CMIP6 will consist of the “runs” from around 100 distinct climate models being produced across 49 different modelling groups.



Say that one wants to use Machine Learning on those results



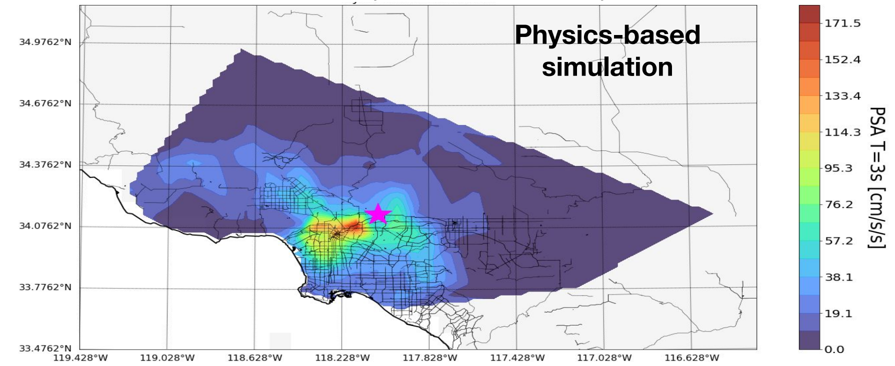
Example 1. The DT-GEO component DTC-E5 (ground shaking simulation)



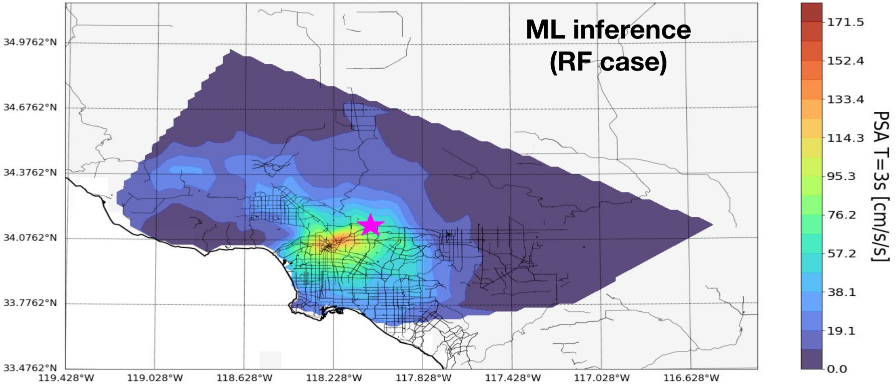
Off-line (HPC component)			Urgent computing
Scenarios (physics-based)	**Data analytics and training**	**ML model evaluation**	**MLESmap**
For example, the CyberShake Study 15.4 (CSS-15.4) for California contains a dataset with 155M of sinthetic events	Training using a Deep Neural Network (DNN) model and a decision-tree model (Random Forest, RF)	Evaluate error statistics depending on earthquake magnitude and target variables	Retrive new earthquake information (real-time) and generate AI-based ground-shaking maps in seconds

Example 1. The DT-GEO component DTC-E5 (ground shaking simulation)

Comparison between HPC physics-based forward simulation and ML inference for an earthquake in the LA metropolitan area



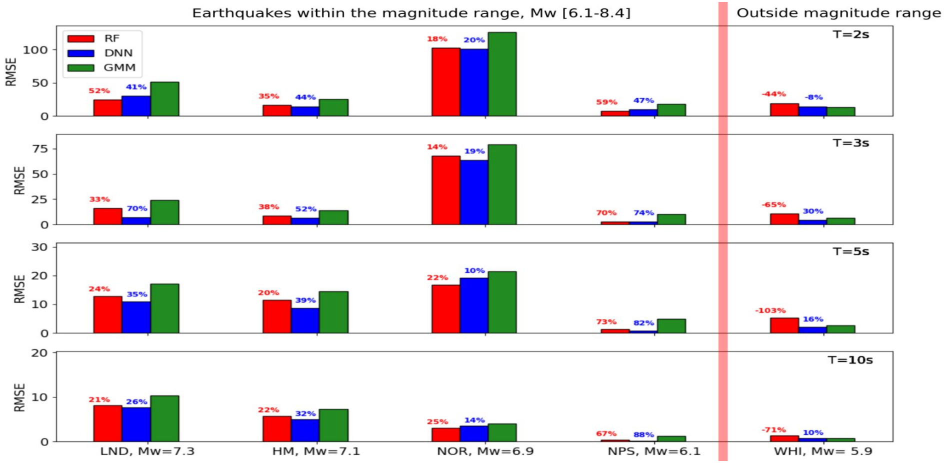
Time-to-solution (minutes to hours)



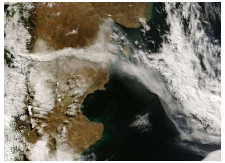
Time-to-solution (seconds)

RMSE validation of ML inferences (DNN and RF) and traditional Ground Motion Models (GMM) approach against real observations from seismographs

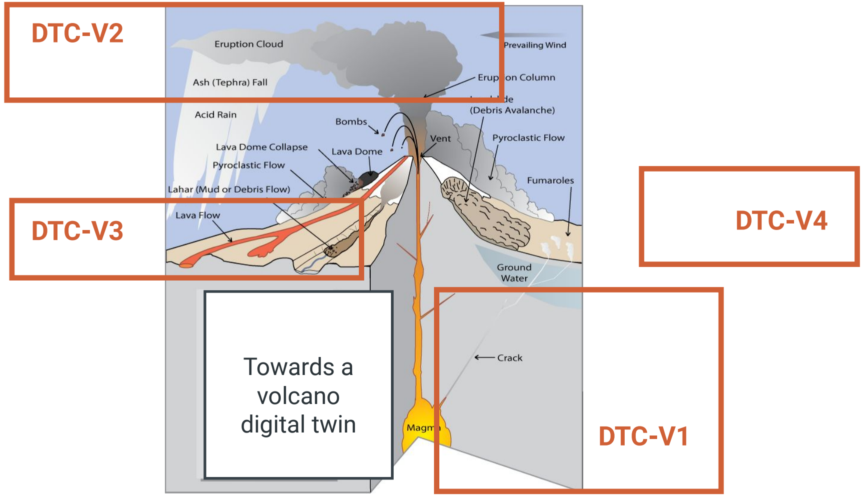
- Left to right: results for 5 past earthquakes of magnitudes 7.3, 7.1, 6.9, 6.1 and 5.9 occurred in the LA basin
- Top to bottom: results for 4 different periods of interest (2s, 3s, 5s, 10s)



Example 2. The DT-GEO component DTC-V2 (volcanic ash dispersal)

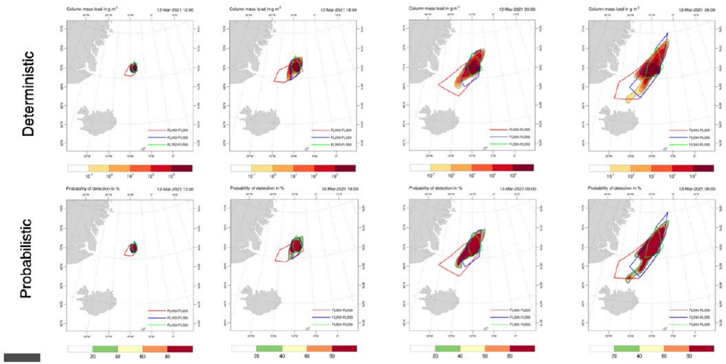


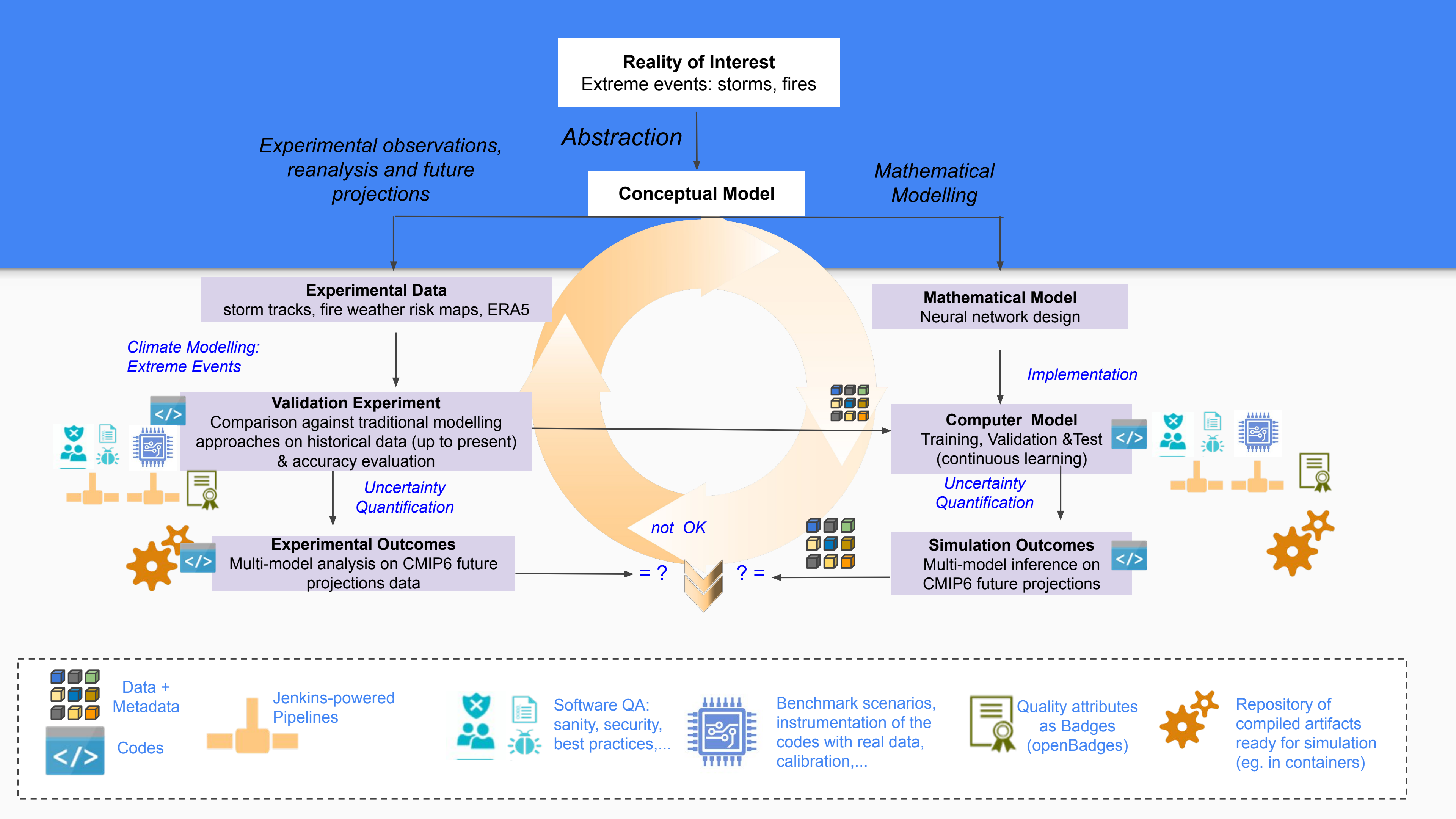
ChEESE



DTC-V2
• Triggered by DTC-V1 and other obeservations • Runs the FALL3D dispersal model to produce urgent computing ensemble-based deterministic and probabilistic forecasts of ash dispersal and fallout • The ensemble members span the range of uncertainties in observations driving the model • Runs on HPC systems (GPUs) • Tailored to civil aviation purposes (avoid airplane encounters)

Digital twin		Impacts	
DTC-V1	Triggers	**DTC-V2**	Ash dispersal
		DTC-V3	Lava flows
		DTC-V4	Gas dispersal
State of the volcano based on geophysical monitoring and models		Urgent computing impact assesment combining physics-based models (HPC) and observations	




Reality of Interest
Extreme events: storms, fires
Abstraction
Experimental observations, reanalysis and future projections
Conceptual Model
Mathematical Modelling
Experimental Data
storm tracks, fire weather risk maps, ERA5
Mathematical Model
Neural network design
Climate Modelling: Extreme Events
Implementation
Validation Experiment
Comparison against traditional modelling approaches on historical data (up to present) & accuracy evaluation
Computer Model
Training, Validation &Test (continuous learning)
Uncertainty Quantification
Uncertainty Quantification
not OK
Experimental Outcomes
Multi-model analysis on CMIP6 future projections data
= ?
? =
Simulation Outcomes
Multi-model inference on CMIP6 future projections
</>
Data + Metadata
Codes
Jenkins-powered Pipelines
Software QA: sanity, security, best practices,...
Benchmark scenarios, instrumentation of the codes with real data, calibration,...
Quality attributes as Badges (openBadges)
Repository of compiled artifacts ready for simulation (eg. in containers)

Approach to developing a Quality framework for DT based on DevOps-oriented technologies

- **DevOps** => movement
  - Improve efficiency reduce time from software development to production
  - Requires heavy automation of the development and delivery process
- **CI/CD** => method
  - Method to release software more frequently, relying on automation
- **Jenkins** => tool
  - Open source CI/CD system for automation to build software, test & deploy
- **Jenkins Pipeline as Code** => implements a process from software testing to delivery
  - Allows building the software in a reliable and repeatable manner
  - Allows to automate the multiple stages of the process from testing to delivery

Technologies and key ideas
(more details in today´s following presentations)

Codes

Data +
Metadata

Benchmark scenarios, instrumentation of the codes with real data, calibration,...

Repository of compiled artifacts ready for simulation
(eg. in containers)

Software QA:
sanity, security, best practices,...

badgr

Quality attributes as Badges
(Synergy Badges)

OSCAR

Serverless,
Real time data

dCache

Jenkins- powered

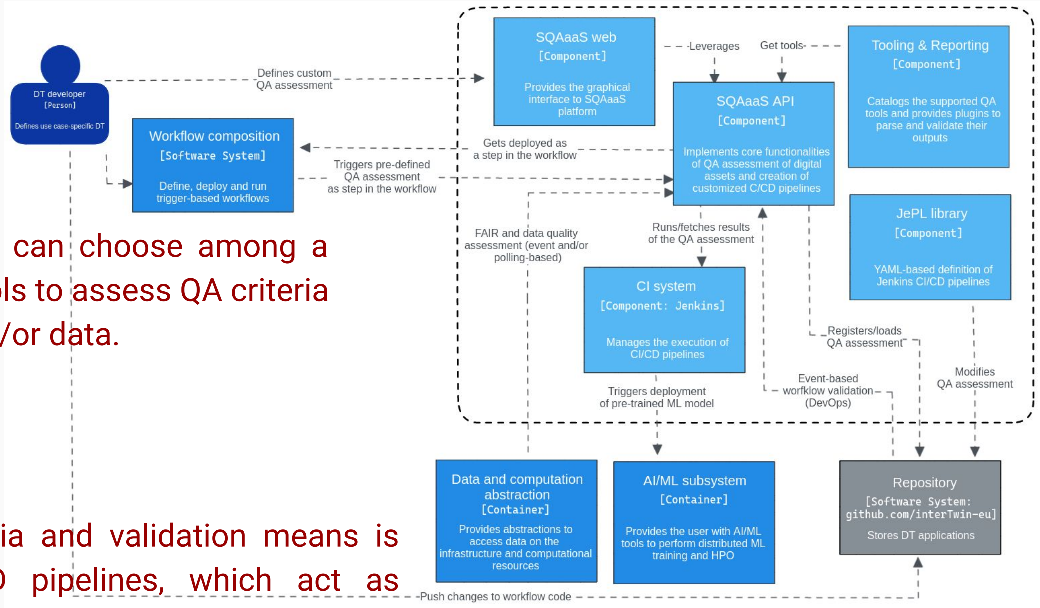
SQAaaS

UDOCKER

docker

Validation/Uncertainty verification as part of ML training workflow via SQAaaS

(3) CI/CD pipelines are triggered on-demand, as the final acceptance check of a pre-trained ML model before moving it to production,



(1) The DT developer can choose among a set of libraries and tools to assess QA criteria relative to models and/or data.

(2) The list of criteria and validation means is wrapped into CI/CD pipelines, which act as quality gates during validation of DT workflows.

(4) CI/CD pipelines also triggered as a response to events: data ingestion systems, or by repository platforms as a result of code changes

Scientific computing has never been “business as usual”

- Not just a ”IT service” but an integral element of research
- Complexity of experimental/observational instruments and size of data volumes

  → more computing power, data storage, computationally expensive algorithms in a funding context of flat budgets

- **Integration of technological solutions** is a must
- **Software and Computing** is a global endeavor: efforts must be coordinated: (heavy work with rare and expensive talents)