

L' Intelligenza Artificiale per accelerare lo sviluppo di tecnologie R&D innovative per la transizione Net-Zero

Francesco Cannarile Roberto Grana <u>Giacom</u>o Gorni

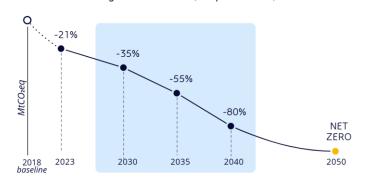
9 Ottobre 2025

This document is the property of Eni, which holds all rights. The material may not be reproduced, distributed, altered or used for purposes other than consultation by webinar participants.

# Digital for R&D: Motivation & Context



Net GHG lifecycle emissions (scope 1+2+3)



- We have embarked on an **industrial transformation** involving all business lines to decarbonize the entire company. To this end, we invest in researching, developing, and implementing **transition technologies**.
- According to the technological neutrality principle, there is no single solution to achieve the energy transition, we need a technological mix that can be adapted to different applications and needs. This is why we are developing a wide range of technologies that support the decarbonisation of each sector of the economy and our daily lives.

## Eni applications in R&D to achieve Net Zero Emission



Energy from renewables

Electric and thermal energy



**Fusion** 

The electricity and thermal energy of tomorrow



Circular Economy

Biofuels, sustainable chemistry and critical materials



**CCUS** 

Decarbonization of processes

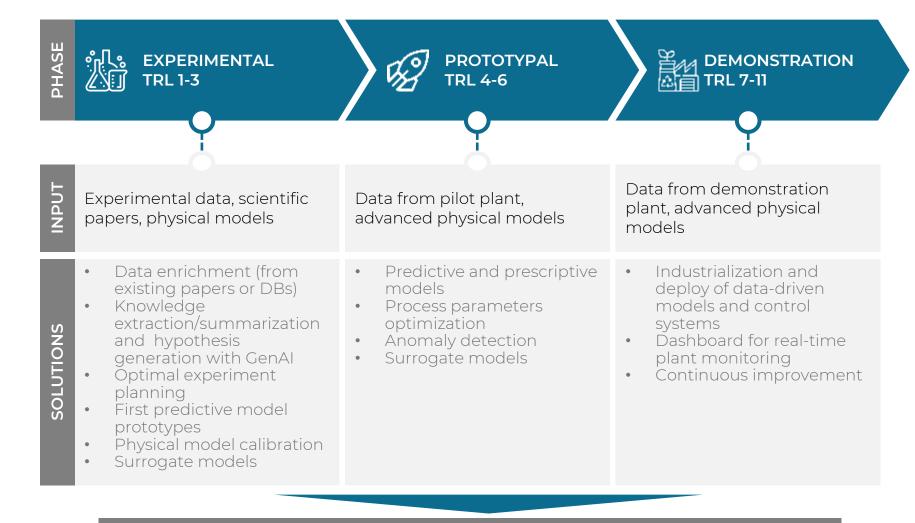


Environment

Ecosystem restoration

## How AI can boost experimentation





Develop a Digital Twin of the plant since the Pilot phase to exploit it in demonstration phase

**Artificial Intelligence** Advanced Modeling & Simulation





# DESCRIPTION

#### **STUDY**

#### **Defining** the problem and desired material properties based on the intended application. Perform literature review and create a first database of material

- **Reviewing** prior research, patents, and material databases to gather relevant insights.
- Extracting and organizing data from existing experimental or computational investigations
- Simulating by first principle methods data set when these are not available or not reliable.

#### **HYPOTHESIZE**

#### Formulating hypothesis and proposing a set of candidate materials with target properties for further evaluation

- Proposing a promising set of candidates for further evaluation via iterative exploration
- Formulating hypotheses using theoretical or computational model chemical physical-based

#### **SCREENING**

#### **Evaluate** material candidates by analyzing their predicted properties and stability, prioritizing those with the highest potential for success in the intended application

- Running computational chemical physical-based models and/or Artificial Intelligence based ones to assess candidates' properties.
  - **Assessing** key factors s by focusing on those with the highest likelihood of success.

#### **TESTING**

Determining synthesis pathways, synthesizing materials, measuring properties at atomic and macroscopic scales, and refining processes based on experimental results

- Extract synthesis recipes from literature (AI) and propose potential routes using advanced computational modeling techniques.
- Analyze experimental data
- Using computational model to validate experimental results

# Example - Al for accelerating carbon capture technologies

Providing real-time and automated

and

**prediction** of

assessment

quantities of interest



Machine

learning

of interest to be monitored

**networks**) model to predict quantity

(deep

## Objective

**PREDICTIVE** 

MODELING

Support research and development in **designing**, **validating** and **industrializing** a **new technology for CO2 capture** through developing **artificial intelligence tools** 

	Objective	Input	Developed solution
FIRST-PRINCIPLES MODELING	Provide a <b>mathematical description</b> of the system behavior for a better understanding of the system and simulate scenarios of interest	<ul> <li>Experimental data</li> <li>Data of literature</li> <li>Subject Matter Experts knowledge</li> </ul>	<ul> <li>First-Principles model based on differential equations that allows simulating the trajectory of an experiment</li> <li>Meta-heuristic optimization algorithms (differential evolution) to calibrate physical model parameters</li> </ul>
OPTIMIZATION AND CONTROL	Prescribing the optimal set-points for the experimental setup in order to performance in real-time	Simulation from the calibrated first- principles model	<ul> <li>Reinforcement learning model to prescribe the best set points for the experimental setup to optimize system performance in real-time using simulations from the first-principles model</li> </ul>

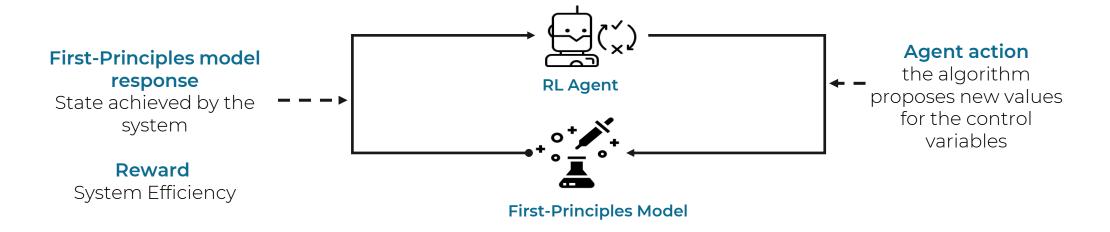
Experimental data

Calibrated first-principles model

# Reinforcement Learning for optimal system control



• Modeling approach: the system is represented by the first-principles model. The agent interacts instant by instant with the first-principles model by proposing new values of the variables to be optimized (actions) and causing the model to evolve (new state) and return a new value of system efficiency\* (reward).



RL Algorithm: Deep Deterministic Policy Gradient (DDPG)

#### Results

System performance obtained with RL is doubled with respect to the not optimized setting



# Focus on Design of Experiment & Optimal Experimental Design

# Why Design of Experiments (DoE)?

#### **CHALLEGE IN R&D**

- Developing new technologies or processes involves many variables
- Resources are limited: experiments cost time, money, and materials.
- Trial-and-error or "one factor at a time" testing is:
  - Too slow
  - Cannot reveal interactions between factors
  - Often gives incomplete or misleading results

#### THE NEED

#### R&D teams require:

- Learning more with fewer experiments.
- **Building** a quantitative understanding of how factors affect outcomes.
- **Predicting** and optimize results before scaling up.

#### THE ANSWER: DOE

- DoE provides a statistical structured approach to experimentation
- Each test is designed to contribute maximum information to the overall picture
- Fewer runs, deeper insights, faster and more reliable decision making

## What is DoE?



# A SMARTER WAY TO EXPERIMENT

- DoE is a **structured method** to plan and run experiments
- Instead of changing one variable at a time, it tests multiple factors together in a systematic way.
- Each experiment is chosen so that, combined with the others, it builds a complete picture of how the system behaves.

# WHAT IT DOES

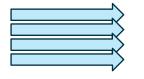
- Identifies the factors that really matter ("vital few")
- Reveals how factors interact (e.g. temperature may matter more at high pressure)
- Builds a predictive model linking inputs
   → outputs
- Helps find the best settings for performance, quality, or cost.

# WHY IT MATTERS

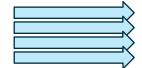
- Saves time and resources by avoiding redundant trials.
- Provides **scientific confidence** instea of guesswork.
- Creates knowledge that can be reused and scaled up.

#### Process/ product

Controllable input variables (X)





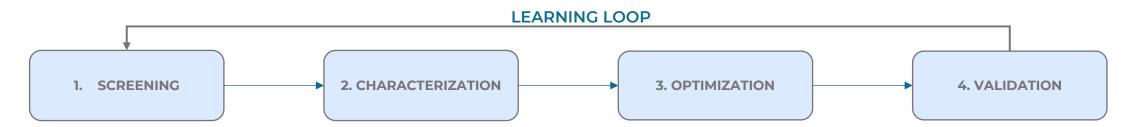


Output variables (Y)

# The DoE Journey



An iterative process where each step builds on the results of the previous one



Efficiently **identify** the most influential factors (the "**vital few**") from a wide range of possibilities. This reduces complexity and focuses subsequent efforts on a smaller, more manageable set of variables.

**Method**: Fractional factorial design (linear screening model)

**Quantify** how significant factors behave collectively by modeling their main effects and, crucially, their interactions. The outcome is a first-pass mathematical model of the process that explains how variables work together.

**Method**: Full factorial design (linear model with interaction terms)

Locate the optimal settings for process variables by modeling response curvature (i.e., quadratic effects). This involves running new, targeted experiments to precisely estimate the factor levels that maximize or minimize the output.

**Method**: Response Surface Methodology (RSM) with quadratic models (CCD, Box-Behnken). Formally **validate** the final model. Use statistical analysis to test the significance of all model terms, then conduct **confirmation runs** to empirically verify the model's predictive accuracy and ensure the results are reproducible

**Method**: Model diagnostics, confirmation runs

# From DoE to Optimal Experimental Design

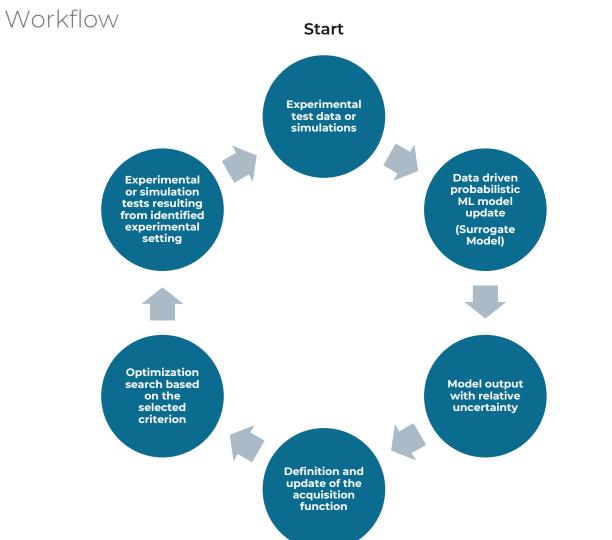


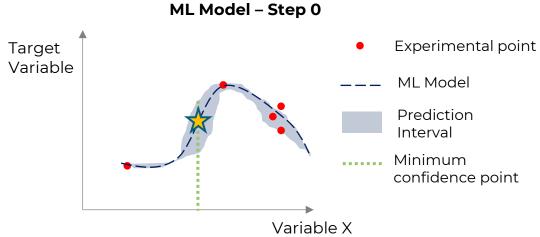
Evolving from a fixed plan to a dynamic learning strategy

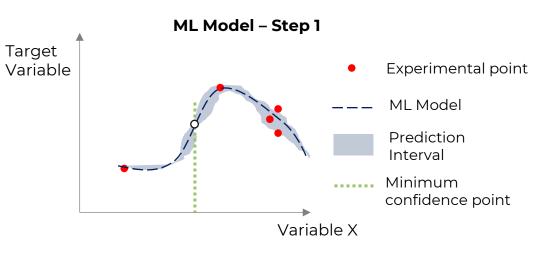
	Classical DoE The statistic blueprint	Optimal Experimental Design  The adaptive strategy		
PLANNING	Fixed and pre-defined (e.g., Factorial).	Model-based and <b>built sequentially</b>		
FLEXIBILITY	All runs are <b>decided upfront</b> with no adaptation (rigid)	Works as a loop in an <b>adaptive way</b> (run → update model → choose next).		
APPLICABILITY	Limited to simple, linear, or polynomial models.	Handles complex, <b>non-linear systems</b> and <b>practical constraints</b> .		
EFFICIENCY	Some tests may bring <b>little</b> new information.	Leads to <b>faster</b> decisions with <b>fewer</b> experiments.		

## **Optimal Experimental Design**









Experimental tests

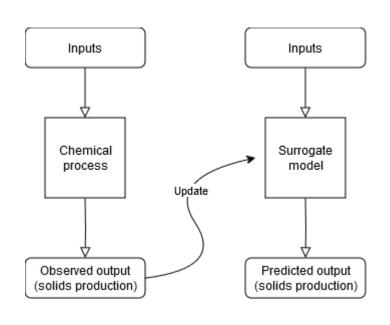
Tests suggested by the OED methodology

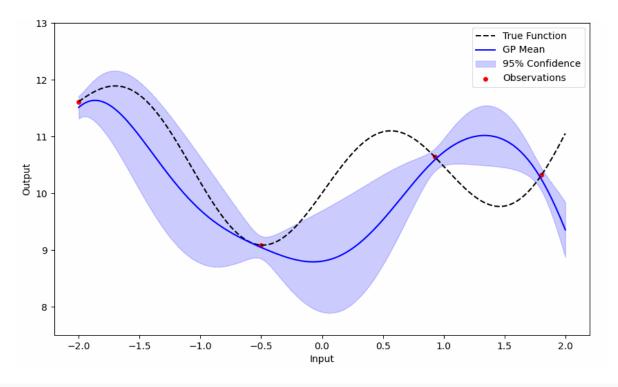
# Surrogate Model - Data driven probabilistic ML model



A probabilistic ML model is used to approximate the unknown process that relates the inputs and the outputs. The model should be able to provide

- 1. A prediction of the output, which is more accurate the more data we have to train the model on
- 2. A prediction interval around the prediction to represent the uncertainty of the model about the prediction





# Making decisions: the acquisition function



An acquisition function defines how to select the inputs for the next experiment. Different acquisition functions allow for different experiment design strategies.

#### **Exploitation**

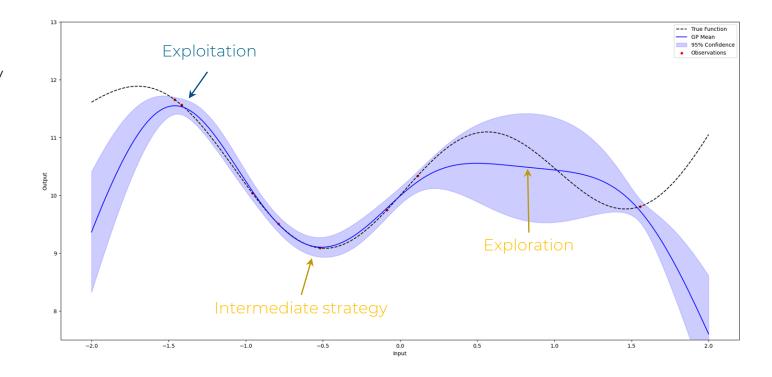
- "Go where we think the best results are"
- Like going down the lowest visible valley

#### **Exploration**

- "Go where we are most uncertain"
- Like mapping unknown territory

## Intermediate strategy

- "Go where we are confident of the best results, but allow some exploration"
- Balances exploration and exploitation

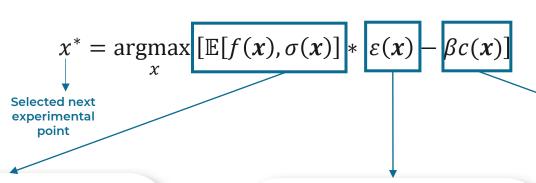


Each acquisition function has its advantages and disadvantages, and its use depends on the objective.

# Choosing the next experiment: the acquisition function



An example of acquisition function



#### **Expected Improvement**

Assigns a **high score** by balancing two strategies: **Exploitation** (leveraging the model's current certainties, testing where it already predicts an optimal outcome) and **Exploration** (investigating uncertain areas that might hide a breakthrough).

#### **Error Reduction**

Gives a **high score** to the experiment that will most reduce the model's overall empirical error. Its goal is to make the model globally **more accurate and trustworthy.** 

#### **Constraints**

Applies a mathematical **penalty factor**, directly lowering the score of any experiment that violates realworld limits (e.g., cost, time, safety).

## The optimization algorithm

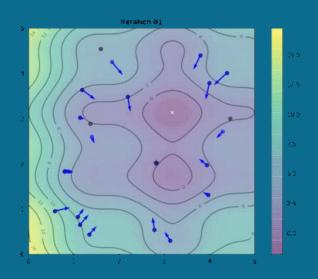
The optimization algorithm is the **numerical solver** that finds the most promising next experiment, given the surrogate model and the acquisition function.

#### **HOW IT WORKS**

- 1. The acquisition function (derived from the surrogate model) defines the objective function **to be optimized**.
- 2. The algorithm **explores** the input space to find its maximum.
- The result is the next experimental point to test.

#### TYPICAL SOLUTION METHODS

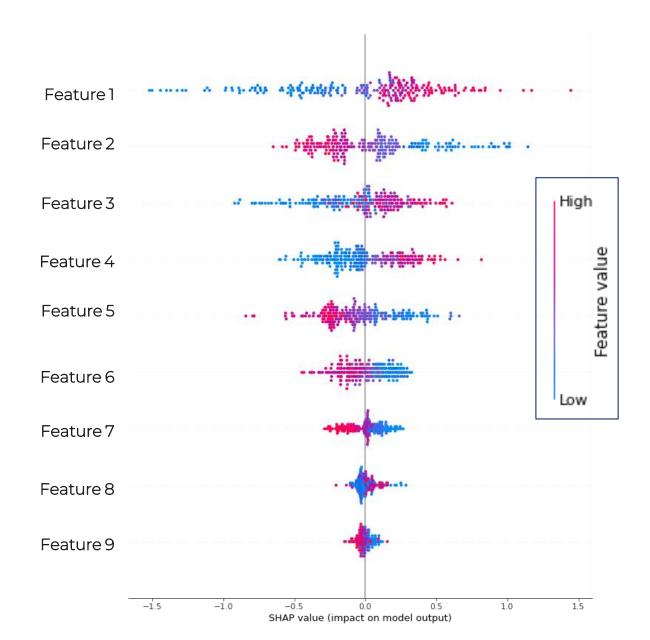
- Gradient-based search: fast if the function is smooth, but may get stuck in local optima.
- **Global search heuristics**: genetic algorithms, simulated annealing, particle swarm slower but robust.
- **Bayesian optimization routines**: combine Gaussian Processes with acquisition functions; popular for expensive experiments.



Example of iterations using metaheuristic optimization (Particle swarm optimization)

## **OED - Feature contribution**





The surrogate mode cab be used to analyze the **most impactful** features of the system and what is their possible effect on the prediction.

**Shapley values** are typically used to infer the feature contribution.

- Feature 1
- Feature 3
- Feature 4
- Feature 8
- Feature 7
- Feature 6
- Feature 9
- Feature 2

Positive impact on target

Negative impact on target



# Optimal Experimental Design in Bio-feedstocks pretreatment processes

## **BioRefining Value Chain**

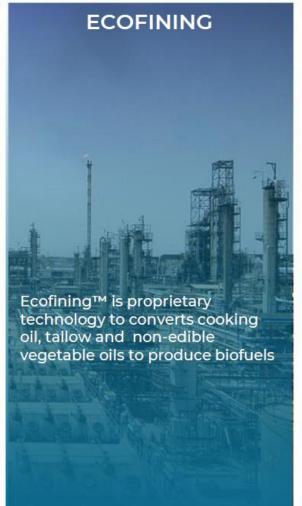
## Enhancing value across processes



- tallow
- waste or used cooking oil (UCO)
- wastes or residues such as nonfood-grade vegetable oils, animal fats, sludge palm oil mill effluent (POME)



Pretreatment unit is necessary to remove impurities such as phosphorous, metals, polyethylene, nitrogen and chlorine-containing components that are naturally present in some raw materials





## **Development of an Unconventional Pretreatment Process**



#### **Definition of UnConventional Bio-Feedstocks**

The unconventional raw bio-feedstocks usually contain high amounts of pollutants such as:

- metals,
- phosphorous,
- salts, etc.

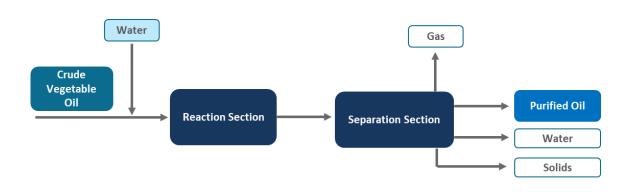


To overcome the conventional pretreatment processes battery limits and to widen the bio-feedstock portfolio, Eni R&D department has developed an innovative pretreatment technology.

#### **Definition of UnConventional Pre-treatment Process**

The unconventional pre-treatment process is based on the right selection of:

- Operating conditions (contact time, temperature, and pressure)
- Ratio between reagents and phases (oil, water, other chemicals agent, etc..)

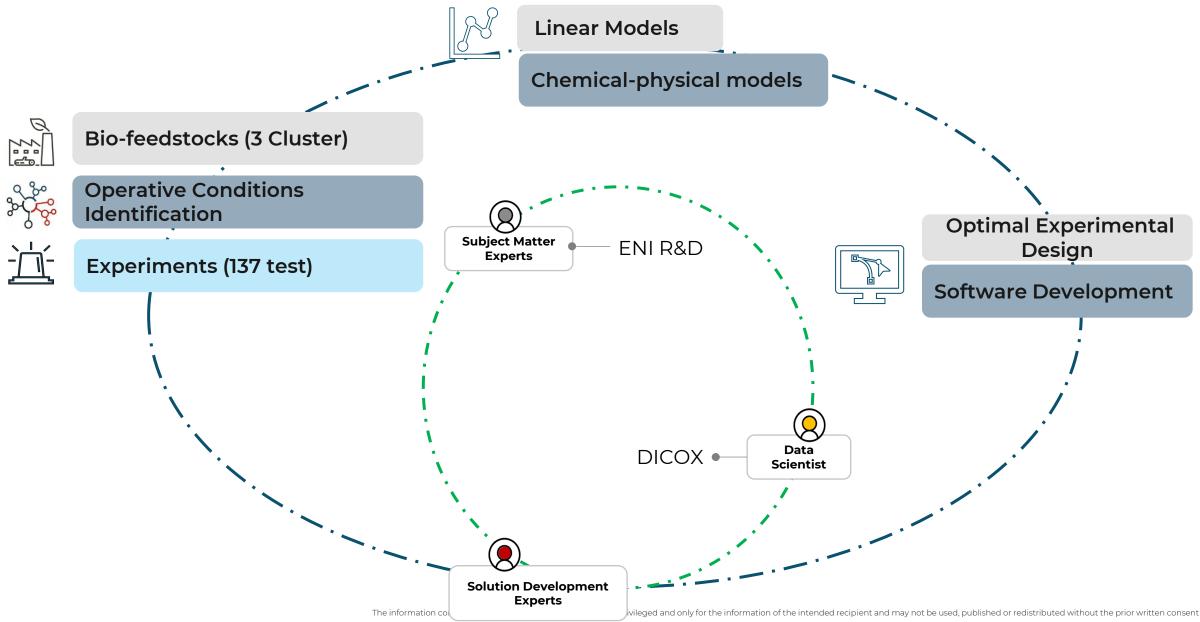


#### The UNCONVENTIONAL pre-treatment has to be:

- Effective in the contaminants removal;
- Simple with low chemical agents e few reaction steps
- Flexible capable to purified a wide range of biofeeds

## **Unconventional Pretreatment Process: Project Team and Workflow**







## Unconventional Pretreatment Process: Digital Boost





#### **Data Aggregation**

Create an experimental dataset and apply advanced analytics techniques to achieve deeper insights and knowledge.



#### Predictive Model and Optimization

Starting from Eni R&D models, develop predictive data-driven linear models to estimate reaction efficiency based on process conditions and bio-feedstock properties



#### Optimal Experimental Design

Apply Optimal Experimental Design techniques to identify new optimal experimental tests based on different criteria



#### <u>Tool Development</u>

Develop a shared tool to allow all R&D users to independently integrate DoE within daily work

#### **Unconventional Pretreatment Process: Data Driven Models**

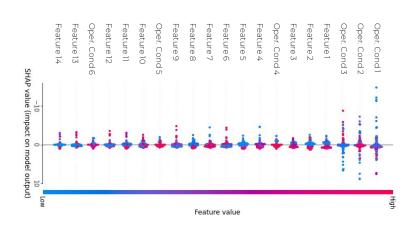


#### **Data Aggregation**

The model shall be fed with proper input data.

#### In details:

- 6 Parameters of process operative conditions
- 17 Parameters of bio-feedstocks (e.g. chemical and physical properties such as acidity, density, carbon %)



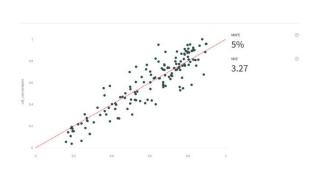
#### At this stage is deemed necessary:

- analysis of input data through ML techniques
- to share main outcomes with the subject experts

#### **Predictive Model and Optimization**

Different strategies have been implemented:

- Different bio-feedstock clustering
- Different predictive models



Campaign	Model	MAE	MSE	
Set 1	linear	0.63	0.72	
Set 2	forest	0.38	0.29	
Set 3	mlp	3.17	28.57	
Set 4	gradient	8.46	152.70	
Set 5	forest	2.11	8.72	
Set 6	gpr	0.80	0.87	
Set 7	forest	2.93	12.66	
Cluster 1	gradient	4.21	59.30	
Cluster 2	forest	2.54	10.04	
Cluster 3	mlp	0.86	2.18	
Multi set	gpr	3.27	42.85	

#### Model training stage:

- Multi-set cluster selected
- Gaussian Process Regressor selected

## Unconventional Pretreatment Process: Optimal Experimental Design (OED)



Optimal Experimental Design goal is to define a new set of experimental test which allow to:

- Filtering inputs relevant to output (screening)
- Build a model to correlates inputs and output (modelling)

In the first stage of analysis, the goals of the experimental investigation shall be defined in order to define the constraints.

The constraints may comprise many aspects, even not strictly related to the technical activity such as time and cost efforts.

#### Selection Criteria

The goal of this specific case study (which is not general) is to minimize the pretreatment efficiency.

In order to have different new experimental points, it was decided to combine points with lower pretreatment efficiency and higher model uncertainty.

For the *Gaussian Process Regressor (GPR)*, model uncertainty is the variance between model predictions and experimental results

## Experimental Design

Parameters	Base Case	EXP1	EXP2	EXP3	EXP 4
Oper Cond 1	0%	-1%	7%	-3%	13%
Oper Cond 2	0%	-41%	-41%	-41%	6%
Oper Cond 3	0%	64%	0%	94%	200%
Oper Cond 4	0%	-6%	25%	25%	25%
Pretreatment Efficiency	0%	14%	-30%	-1%	-11%
Standard Deviation	0%	-72%	-68%	-37%	-45%

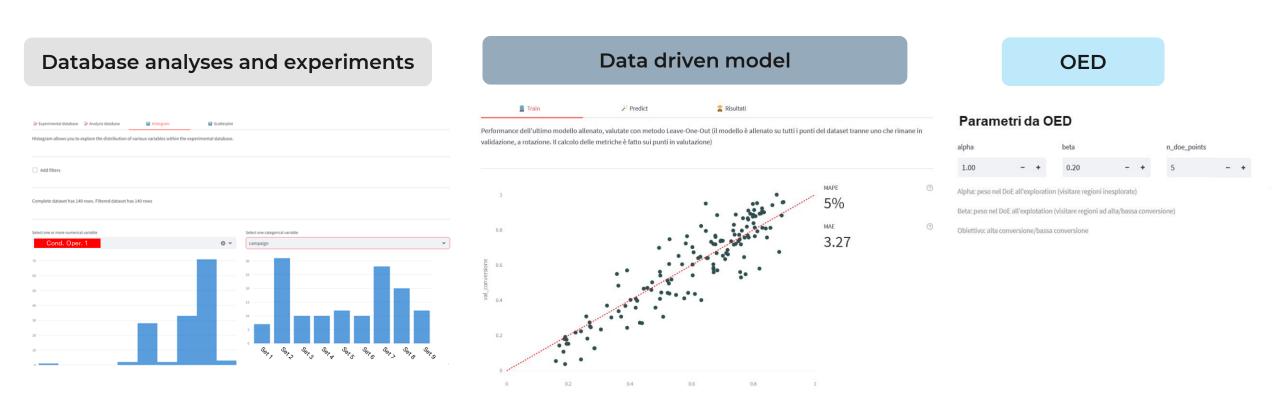
- The new experiments are defined through the OED procedure based on:
  - **✓** Criterion 1: efficiency minimization
  - ✓ Criterion 2: maximum model uncertainty

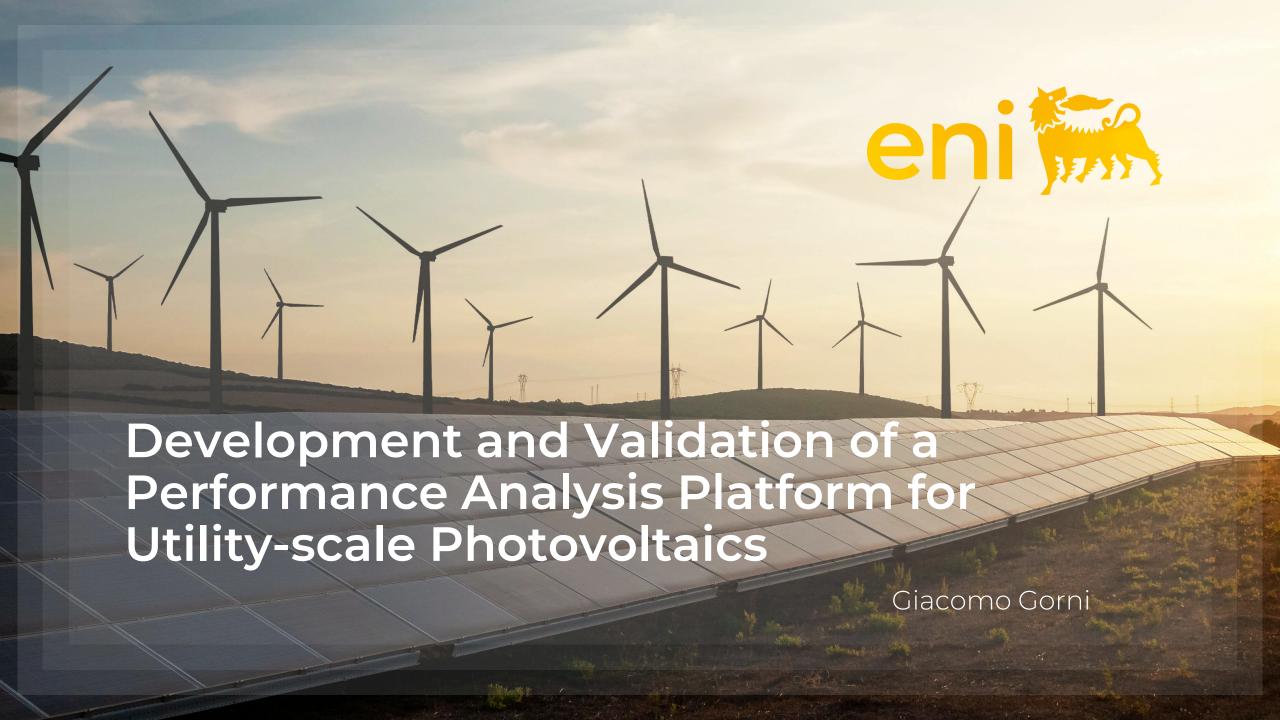
#### **Unconventional Pretreatment Process: Web APP**



The final stage is the development of a tool (Web APP) with the features:

- Collection, management and aggregation of experimental data (database);
- Prediction by the data driven model of new experimental data;
- Application of Optimal Experimental Design to efficiently boost the entire development process by means of upgrading the predictive model.





## Introduction



## **Objective:**

- Reduce capacity downtime
- Speed up underperformance detection
- Speed up O&M troubleshooting

#### **Problem:**

- Multiple masking factors overlapping
- Handle 100ks of data points per plant each day
- Utility-scale PV are huge

#### Solution:

- Identify where the losses are located
- Categorize and rank issues
- Fully automatized process
- User-friendly application

## Methodology Adopted

From a "basic" performance monitoring at plant level

$$PR \propto \frac{Production}{Insolation \cdot Capacity (DC)}$$



To a set of Key Performance Indicators dedicated to main devices (inverters, trackers, combiner boxes)

- Automatically calculated
- Cleared of all the masking factors
  - Comprehensive of suggested corrective actions

# Scale problem

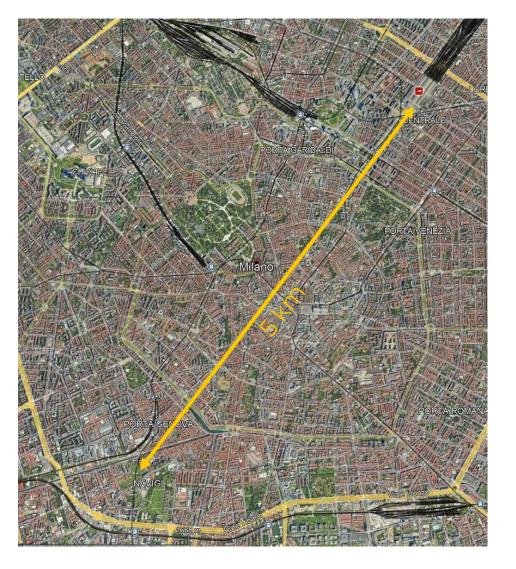


#### Milano

## Utility-scale plant

- 250 MW
- 60 inverters
- 1000 CBs
- 500,000 modules
- 2,500,000 m<sup>2</sup>
- 3000 signals/plant
- 1.7 million datapoints/day





# Traditional monitoring tools

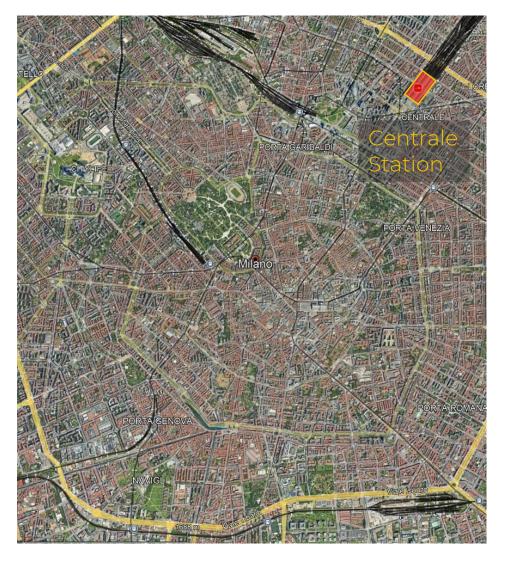


## Milano

## Inverter

- 4 MW
- 16 CBs
- 8,000 modules
- 40,000 m<sup>2</sup>



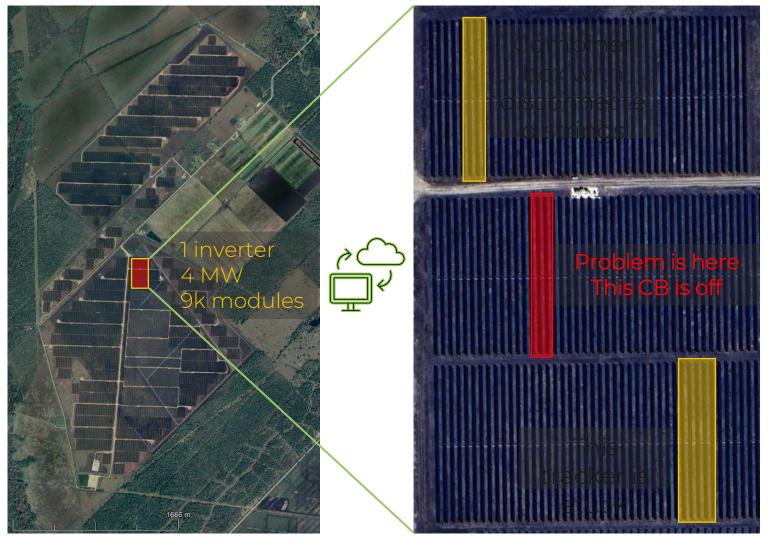


# Digital tools as a solution to the scale problem



## Combiner box

- 250 kW
- ~20 strings
- 500 modules
- 2,500 m<sup>2</sup>



From the MW scale...

...to the 100s kW scale

# Data quality and event labeling



Data analytics tools (AI, ML, physical models...) give access to a solid data quality preprocessing and event labeling.

Plant metadata (GPS, nominal power, layout...)

Actual Weather data (Temp, Irr, Wind, RH...)

Actual production data (power, current, voltage...)



Reconstruct normal behaviour model (Digital Twin expected production output, ...)

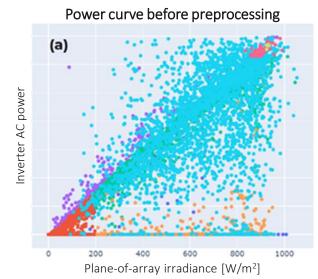
Anomaly identification, quantification, categorization

# Data quality and event labeling

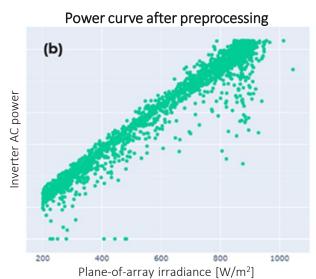


Data analytics tools (AI, ML, physical models...) give access to a solid data quality preprocessing and event labeling.

- Irradiance sensors anomalies.
- MPP deviations (technical or economical curtailment).
- Tracker's wind stow mode.
- Temperature derating.
- Rear Irradiance correction for bifacial systems.
- Tilted irradiance correction by angular response.
- Interrow self-shading effects.
- Inverter clipping detection and correction.







# **Key Performance Inidicators (KPIs)**





### "Advanced" PR

#### Target:

Inverter

Comprehensive metric to have a bird-eye view of the macro trends occurring in the plant.



## DC power health

#### Target:

Combiner box

#### Detectable issues:

- CB off / unavailable
- Non-communication
- Disconnected strings
- Modules degradation
- Misalignment with asbuilt documentation



#### **Tracker health**

#### Target:

Motor

#### Detectable issues:

- Non-communication
- Stalled trackers
- Suboptimal angle
- Wind stow position



## **DC-AC** health

#### Target:

Inverter

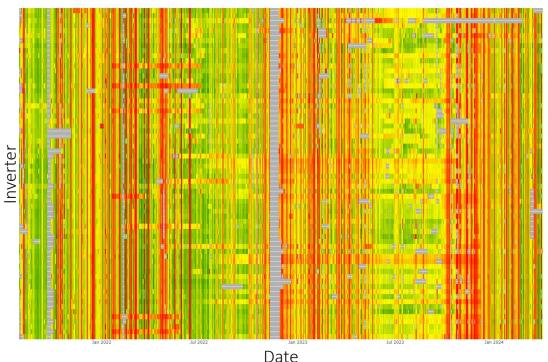
#### Detectable issues:

- Inverter off / unavailable
- Non-communication
- Low efficiency
- Derating

# **KPIs developed – Performance Ratio (PR)**

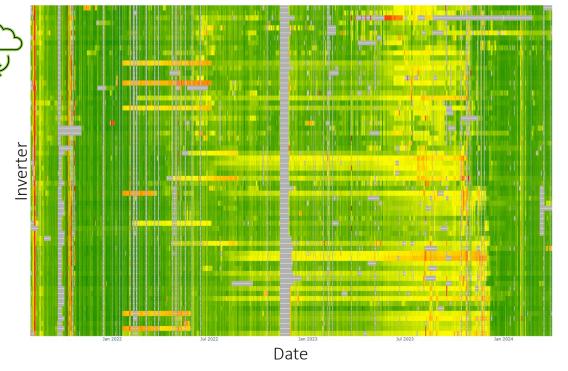






 Any possible underlying issue is masked by a heavy curtailment from the grid operator that artificially reduced the daily standard PR

### "Advanced" Performance Ratio – Inverter level

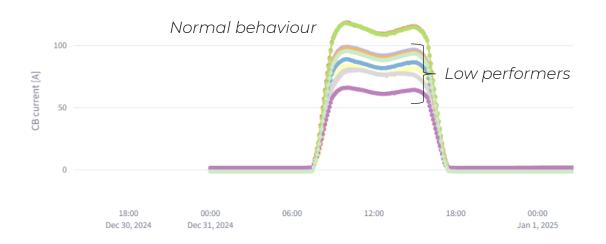


- Results are clearer and more reliable
- Specific pattern have completely different meaning
- Helpful in understanding the more affected areas

# From detailed "top-down" Data Analytics...

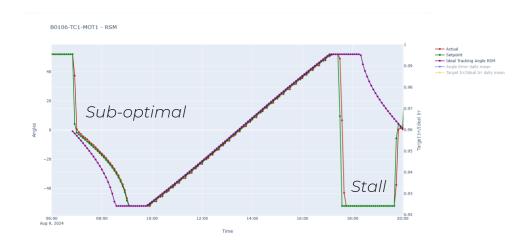


DC power - Combiner Box level



- DC capacity at each Combiner Box (CB) is regressively fitted and normalized to actual weather data.
- A daily peer-to-peer CB comparison identifies underperformers.

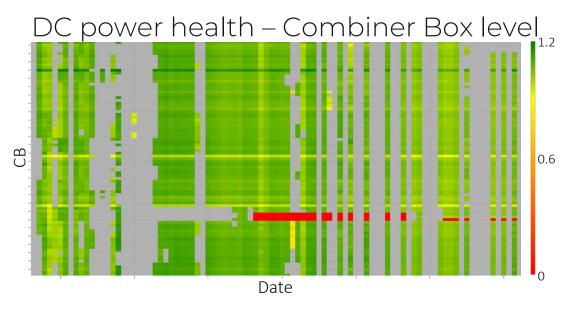
## Tracker angles – Motor level



- Captured irradiance at each tracker is compared to the optimal under ideal orientation.
- A daily analysis identifies setpoint issues (i.e., software) and actual angle issues (i.e., mechanical).

# ... to "bottom-up" new compact KPIs

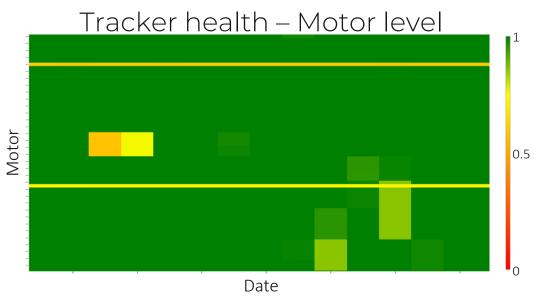




Information at the 100s kW scale

Clear anomaly identification:

- CB off (red)
- Disconnected strings (yellow)
- More strings than as-built (dark green)



Information at the 100s kW scale

Clear anomaly identification:

- Stalled trackers (continuous yellow/orange)
- Ongoing maintenance activities (yellow/orange spots)

# KPIs cross analysis

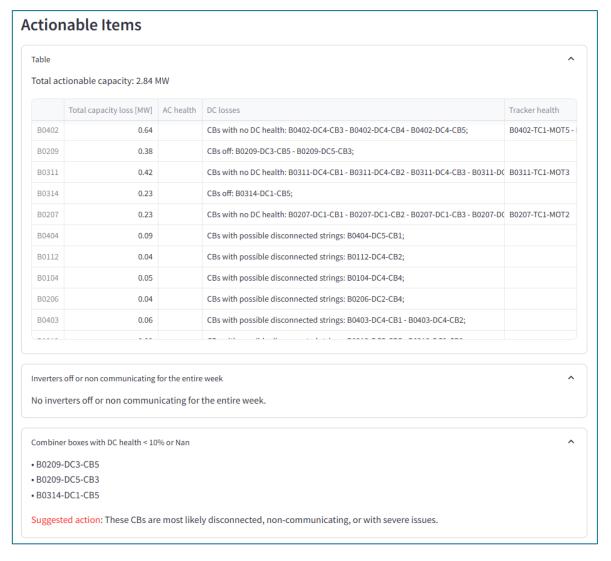
## Comparing KPIs at inverter level:

- Immediate imputation of the loss category and identification of the anomalous equipment
- Verification over time of the effectiveness of the corrective actions



# **Automated Weekly Reporting**



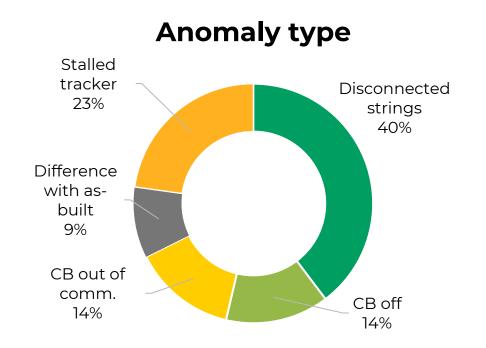


- Every week report only the outstanding anomalies.
- Quantify the anomalies in terms of potential capacity lost to prioritize the activities.
- Clearly list the devices on which the O&M need to focus their inspections.
- Suggest possible root causes.
- Interactive and downloadable.
- Faster transition from the analysis of the anomalies to the action on site.

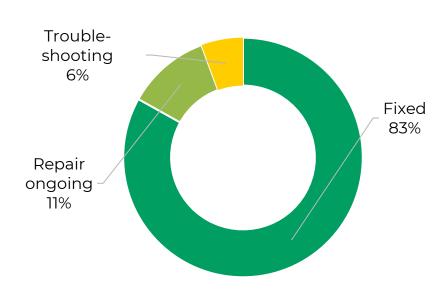
## Results



- Platform deployed on 4 assets
- DC Capacity monitored: ~ 650 MW
- Technologies: mono and bifacial; c-Si and CdTe; back-tracking and true-tracking
- Anomalies identified (Nov 2024 Feb 2025): ~140
- No false positives so far



## **Resolution status**



## Conclusion



- Developed and validated on ~650 MW a digital platform designed to enhance the performance monitoring of large-scale PV plants.
- Preprocessing and data filtering via physics-driven and data-driven algorithms is key to obtain clear and reliable technical KPIs.
- KPIs designed to analyze specific devices and phenomena enabling faster troubleshooting and issue resolution.
- No false positives after four months since deployment.

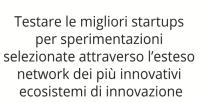
# **Open Innovation**



#### Le nostre iniziative di Open Innovation

Valorizziamo idee, progetti e tecnologie per trovare le migliori soluzioni a livello globale. L'approccio Eni all'Open Innovation prevede attività diversificate con 4 entità:







Programma di accelerazione e sviluppo imprenditorialità

Supportare idee, strategie e percorsi di crescita delle startup

Visita il sito 🖸





Corporate Venture Builder (CVB)

Costruire nuove imprese valorizzando le tecnologie di Eni

Visita il sito 🖸





Corporate Venture Capital (CVC)

Investire in startup per lo sviluppo di tecnologie strategiche

Visita il sito

For more details, please visit

https://www.eni.com/it-IT/azioni/innovazione-tecnologica-collaborazioni/open-innovation.html