



FIT-4-NMP

Strategic and targeted support
to incentivise talented newcomers
to NMP projects under Horizon Europe

HIGH-PERFORMANCE and SUSTAINABLE COMPOSITES INNOVATION WORKSHOP TU DRESDEN 13-14.10.2022

Łukasiewicz - Poznan Institute of Technology – AI Lab

Andrzej Szwabe, PhD

Poland

(potential leader of “an AI-centric / AI-related WP”)

An extended version of the slides is available [here](#).



This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 958255

HI-PERF. & S. C. I. WORKSHOP TU DRESDEN 13-14.10.2022

ABOUT PIT AND MYSELF

- Łukasiewicz – Poznański Instytut Technologiczny (PIT):
Multidisciplinary R&D on the map of **Poznań** and Poland
- Andrzej Szwabe, PhD (PIT **Artificial Intelligence** Lead)



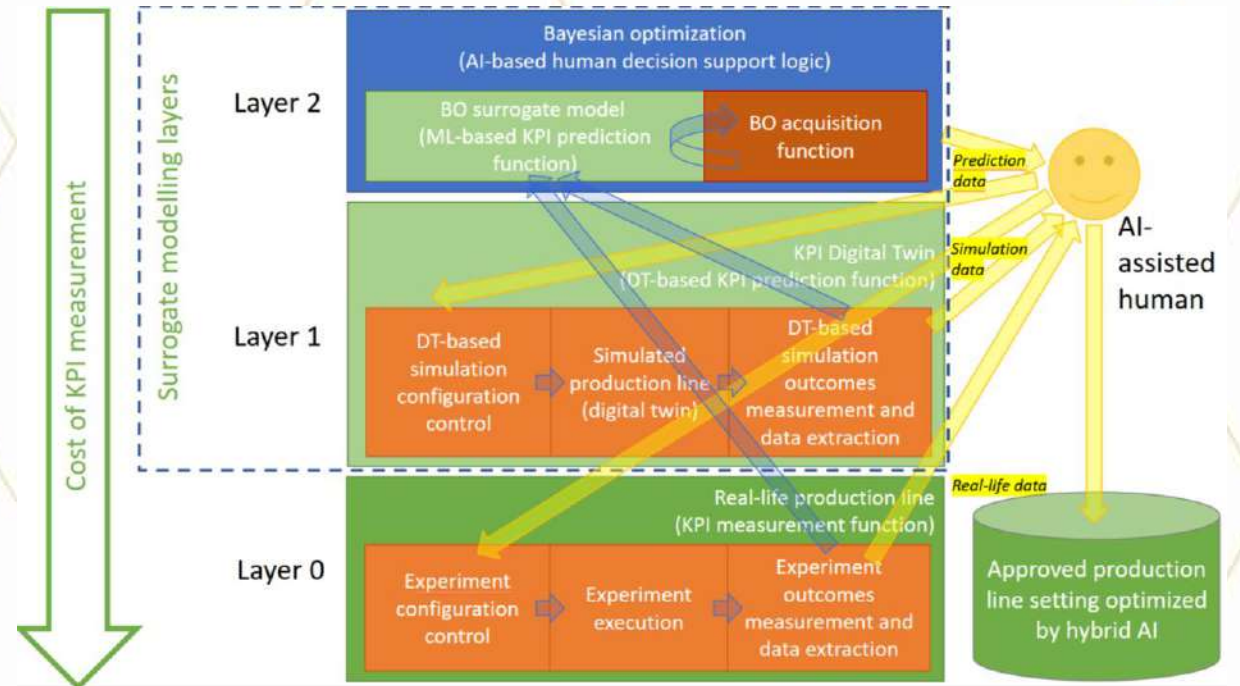
- 10+ years of experience as project manager, data scientists, Machine Learning engineer and Python programmer in 10+ projects with EU universities and companies - Deutsche Telekom, Telefonica, Thomson/Technicolor, INRIA Univ. of Ulm and Freie Univ. Berlin (EU FP6, EU FP7 and Swiss Contribution) of a budget of EUR 10+ million
- Leader of AI/ML development teams at SMEs (KogniTek, Deep.BI, Rogoż, Softhis)
- AI consultant for SwiftShift (USA), Pivotal, KPMG, ERC Venture Capital
- Assistant Prof., PM, ML sys. architect, senior ML soft dev at Poznań University of Technology, Lab of **Intelligent Decision Support Systems**



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HORIZON-CL4-2023-TWIN-TRANSITION-01-31: OUR KEY IDEA FOR CONTRIBUTION TO A PROJECT

- Assumption: In the process of **optimization of production line setting** targeting **energy efficiency** factors such as material design/composition, processing/manufacturing conditions and other **factors of significant impact on the KPIs** may be **modelled as a digital twin (DT) and then reliably simulated**.
- A digital twin applied in a project will enable high-fidelity simulations of manufacturing processes.
- The concept of extended **KPI-estimating digital twin (KPI-DT)** is based on an additional assumption that such a **KPI-DT will enable reliable simulation-based estimation of the key properties of the outcomes/products of the production line and the manufacturing process itself** – both the physical properties and the business KPIs.
 - The idea of KPI-DT is basically an answer to the fundamental question: "How to trade cost-efficiency of DT development for DT-based simulation gap reduction?"

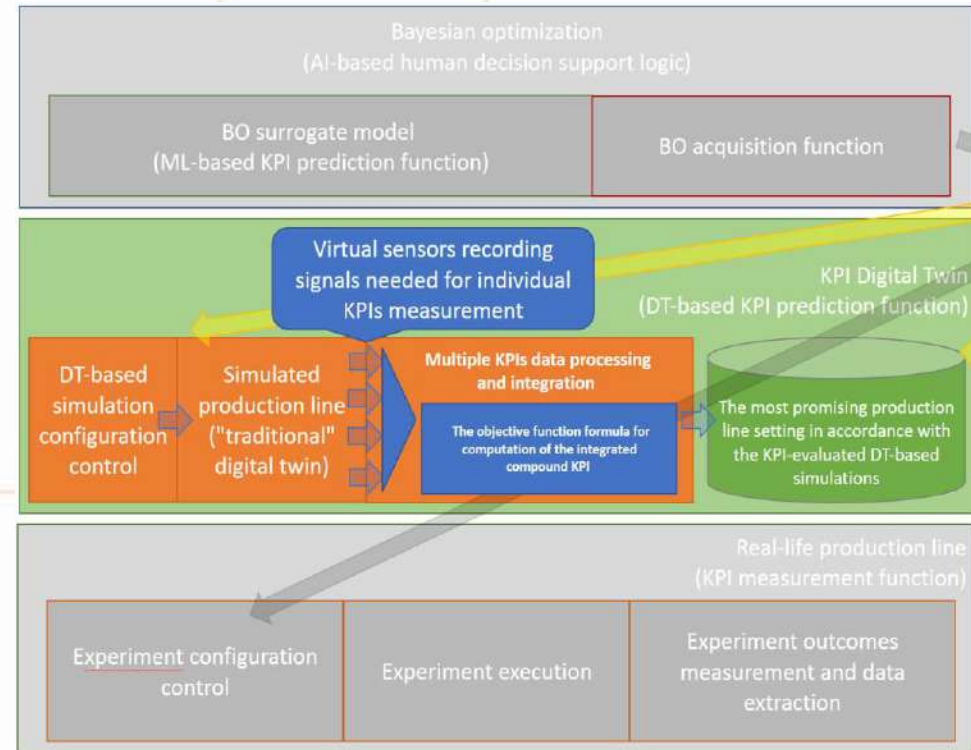


- One of the project outcomes:** AI technology assisting human experts in energy-intensive industry processes optimisation based on an innovative two-layer surrogating architecture. Enhancing KPI-centric digital twin simulations management by non-standard Bayesian optimization will make the industry process optimization more effectively targeting the energy efficiency when compared to optimisation based on "traditional" digital twin simulations not guided by the AI solutions to be developed in the project.



HORIZON-CL4-2023-TWIN-TRANSITION-01-31: OUR KEY IDEA FOR CONTRIBUTION TO A PROJECT

- Thanks to the novel concept of double-level surrogating – combination of **Bayesian optimization** surrogate modelling and **Digital Twin** modelling - **Industry 4.0 processes optimization will become more effective and efficient.**
- The use of advanced BO will allow for extremely efficient search for the optimal settings of the parameters that are relevant from the perspective of "short-term monetary" KPIs (e.g. gross profit, energy consumption cost) and KPIs reflecting safety and economic sustainability.
- Application of the double-level surrogating will make the AI-assisted optimization less dependent on time-consuming and error-prone human work.
- More details may be found [here](#).
- A few partners is interested in joining a HE project implementing the idea: Adam Schmidt (TNO, NL), Mikkel Labori Olsen (DTI, DK), André Meyer-Vitali (DFKI, DE).



- PESA (PL) - PIT's partner and one of the largest producer of rolling stock in EU - is also potentially interested in joining the initiative.

TNO innovation for life

DANISH TECHNOLOGICAL INSTITUTE

DFKI

pesa

PESA Bydgoszcz S.A.
<http://www.pesa.pl>

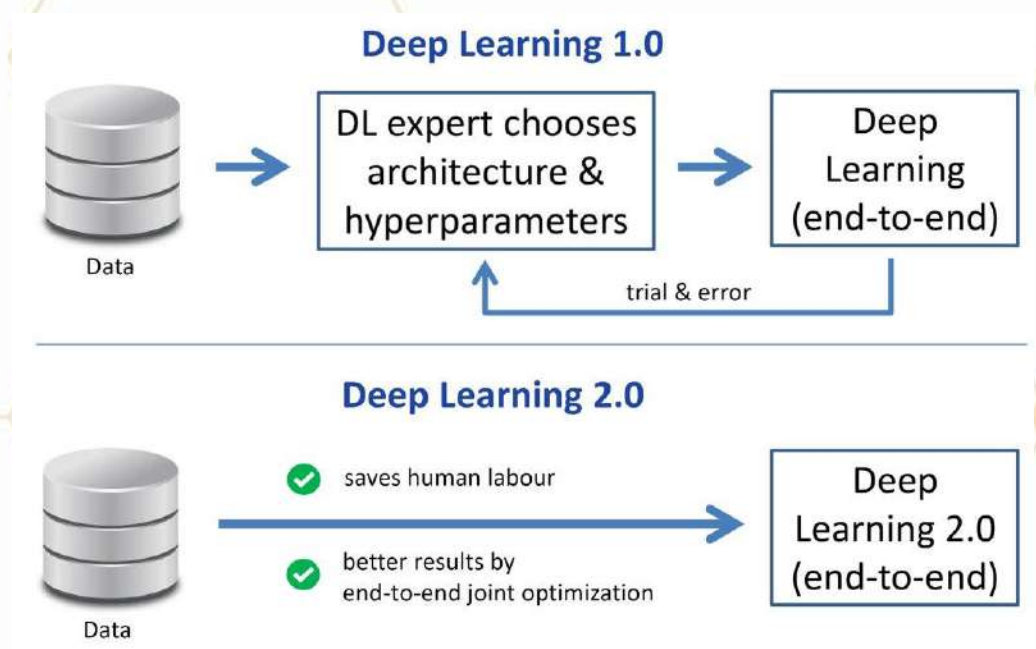


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HORIZON-CL4-2023-TWIN-TRANSITION-01-31: RELEVANT PIT AI LAB TEAM COMPETENCES

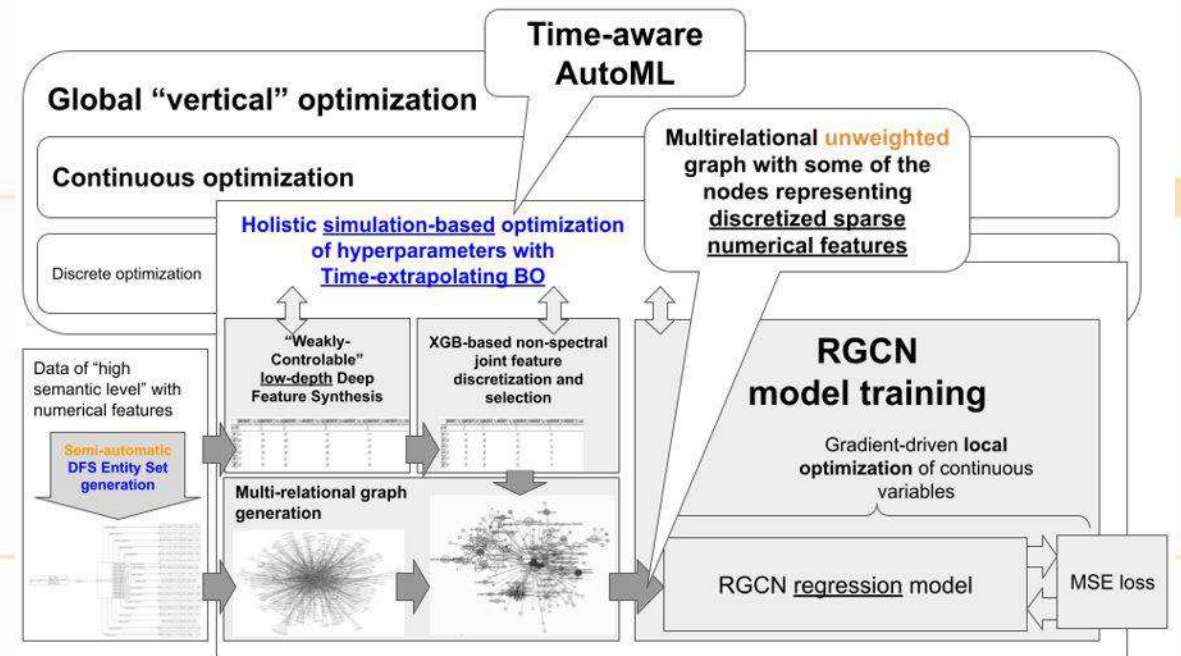
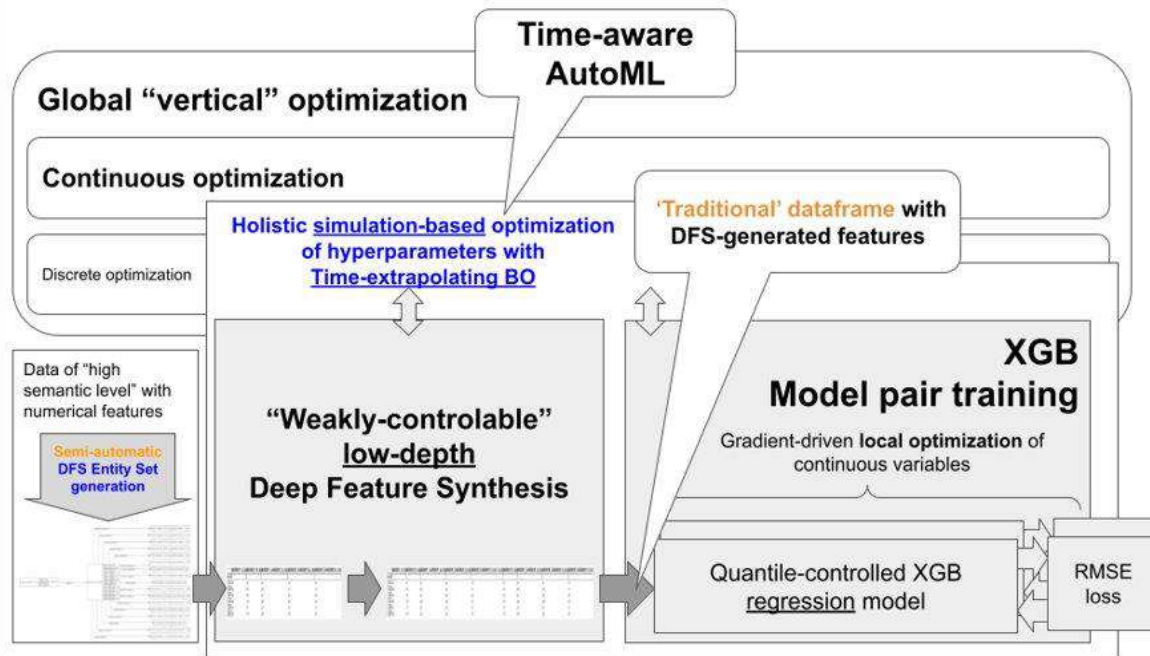
- Full orientation of the AI / ML platform on the optimization of KPIs of a given company.
- Extensive experience in "optimization via machine learning prediction", including Bayesian optimization based on Gaussian process regression, but also on alternative BO-ready regression algorithms.
- Full automation (end-to-end) of fully production-grade machine learning pipelines (end-to-end AutoML, "Deep Learning 2.0" *).
- The highest currently available accuracy of KPIs prediction on business data (relational / tabular: transactional, behavioral, etc.).
- The highest prediction performance currently available on production on microservice Big Data platforms - thanks to "3D scalability" and end-to-end AutoML.

* "Deep Learning 2.0: Extending the Power of Deep Learning to the Meta-Level", Frank Hutter, 2022, <https://www.automl.org/deep-learning-2-0-extending-the-power-of-deep-learning-to-the-meta-level/>



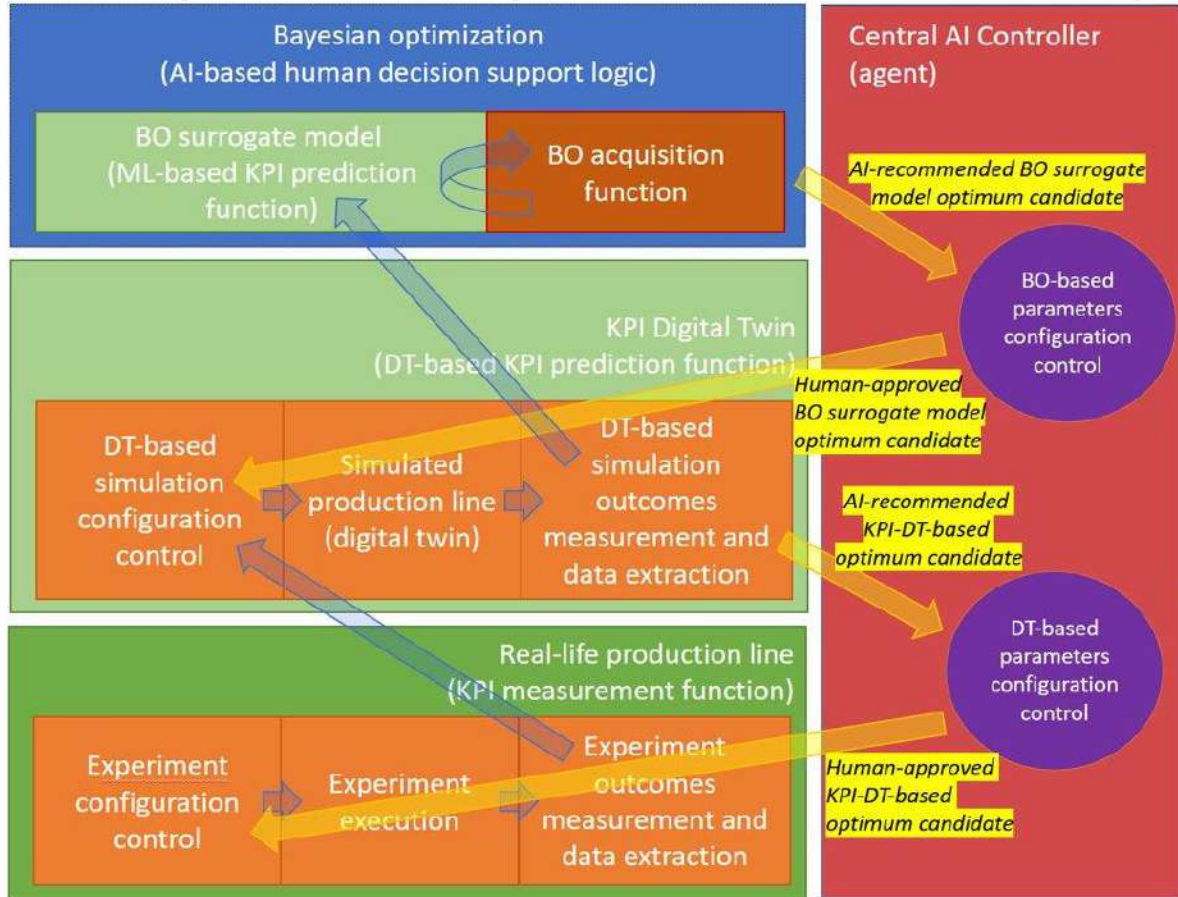
HORIZON-CL4-2023-TWIN-TRANSITION-01-31: RELEVANT PIT AI LAB TEAM COMPETENCES

- Deep knowledge of the latest technologies enabling accurate prediction and optimization of KPIs using business data (relational / tabular: transactional, behavioral, etc.):
 - BI KPI optimization through ML prediction: "which business element to modify to maximize profit"



HORIZON-CL4-2024-RESILIENCE-01-24:

OUR KEY IDEA FOR CONTRIBUTION TO A PROJECT

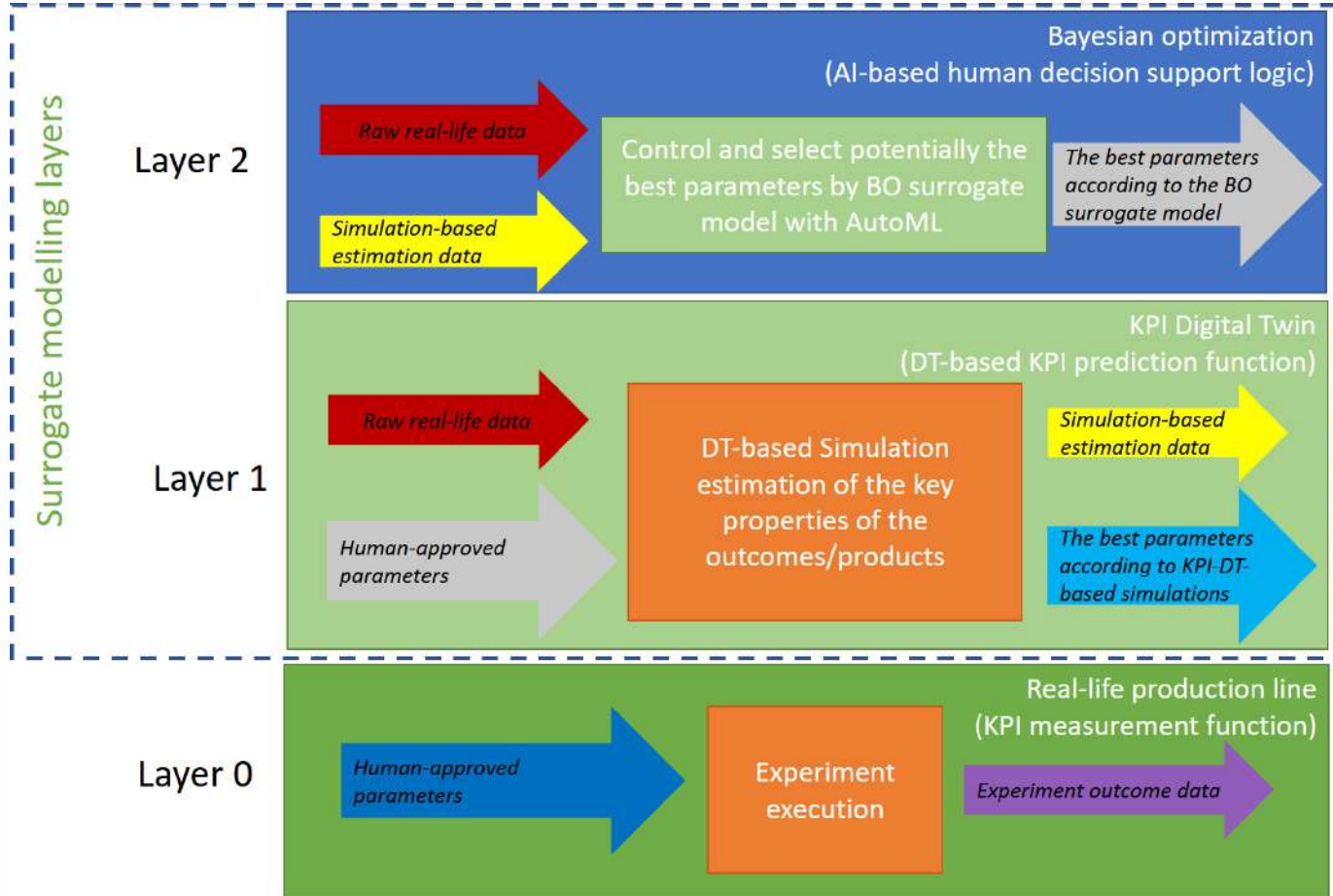


- Our idea applicable in this project is more focused on AI assistance to human expert than on "automated discovery".
 - Human expert controls the selective use of parameters sets recommended by BO.
- At the BO layer, both real-life performance data and simulation performance data is used to update/optimize the BO surrogate model.
 - **BO function ensuring the right balance between the so-called exploration and exploitation is used to produce new production line settings candidates/recommendations.**
 - These recommendations may be used by a human expert as the next production line settings to evaluate at the DT layer.
 - Only the BO layer is capable to automatically use the performance data, as the use of this type of data at the DT layer requires untrivial, manual modifications in the course of the DT development process.



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HORIZON-CL4-2024-RESILIENCE-01-24: OUR KEY IDEA FOR CONTRIBUTION TO A PROJECT



- Each DT-based simulation is executed:
 - to obtain another "promising, hypothetical" performance data point/record that is more reliable than the corresponding objective function value (scalar) prediction realized by means of the BO surrogate model
 - or to obtain another set of simulated time series representing the key properties of the outcomes/products of the production line – both the physical properties and the business KPIs - that may be used to evaluate and analyze the reliability of the DT
- KPI-DT development is realized in cycles corresponding to the growth of the real-life experiment results data set.
 - This development is guided by the unique KPIs-oriented approach to DT evaluation - involving the use of all of the KPIs, not only the single final KPI representing the optimization objective.



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HORIZON-CL4-2024-RESILIENCE-01-24: MOTIVATION AND RELEVANT COMPETENCES OF PIT AI LAB

- The envisioned project involves research on AI-assisted discovery of new materials based on novel Bayesian optimization solutions – in particular on the paradigm of model ensembling innovatively applied to new, structure-aware deep learning algorithms such as **Relational Graph Convolutional Neural Networks - one of the core areas of PIT AI Lab expertise ("semantic / multi-relational deep learning")**.
- It is assumed that the project will be based on two key elements:
 - **Bayesian optimization (BO)** capable to **exploit rich multi-relational semantics of heterogenous data representing various properties of both the materials and the processes of their production - one of the core areas of PIT AI Lab expertise**
 - **Double-layer surrogate modelling** - enabling extremely efficient realization of the so-called objective function evaluations (the key iterative procedure of any AI-assisted material design discovery process) thanks to reduction of the computational costs of unsuccessful digital twin simulations (effectively surrogated by digital twin simulations) in addition to reduction of the costs of unsuccessful real-world material production experiments (surrogated by BO model predictions and/or digital twin simulations)
- More details may be found in [here](#).
- **One of the project outcomes:** AI technology assisting human experts in development/discovery of safe and sustainable materials of reduced substitution barriers based on an innovative two-layer surrogating architecture. Enhancing KPI-centric digital twin simulations management by non-standard Bayesian optimization will reduce the number of experiments necessary to discover a safer and/or more sustainable when compared to "traditional" experimentation not guided by the AI solutions to be developed in the project.



HORIZON-CL4-2024-RESILIENCE-01-24: MOTIVATION AND RELEVANT COMPETENCES OF PIT AI LAB

- To summarize, the team has strong expertise in the following areas of artificial intelligence:
 - Domain-specific, non-standard Bayesian optimization
 - Direct (explicit) KPI maximization via optimization based on machine learning
 - Next-generation time series forecasting based on machine learning
 - Modern end-to-end machine learning automation (a.k.a. Deep Learning 2.0)



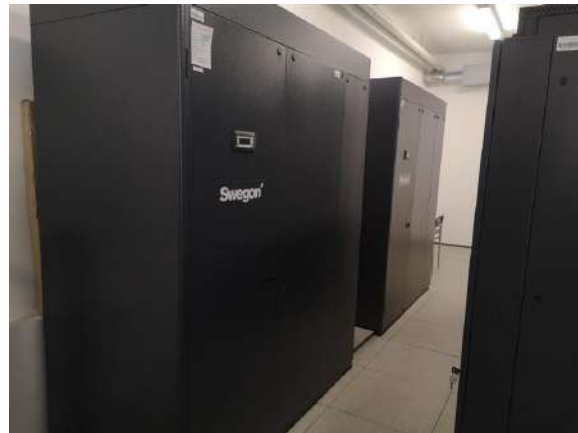
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HORIZON-CL4-2023-TWIN-TRANSITION-01-31

HORIZON-CL4-2024-RESILIENCE-01-24

RELEVANT EQUIPMENT AND FACILITIES

- PIT has 11 physical servers of the following parameters (aggregated):
 - 4 TB RAM
 - 244 CPU cores
 - 70 TB of disk space



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