# Overview of Artificial Intelligence and Machine Learning at SOLEIL

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# Contents

# Artificial Intelligence

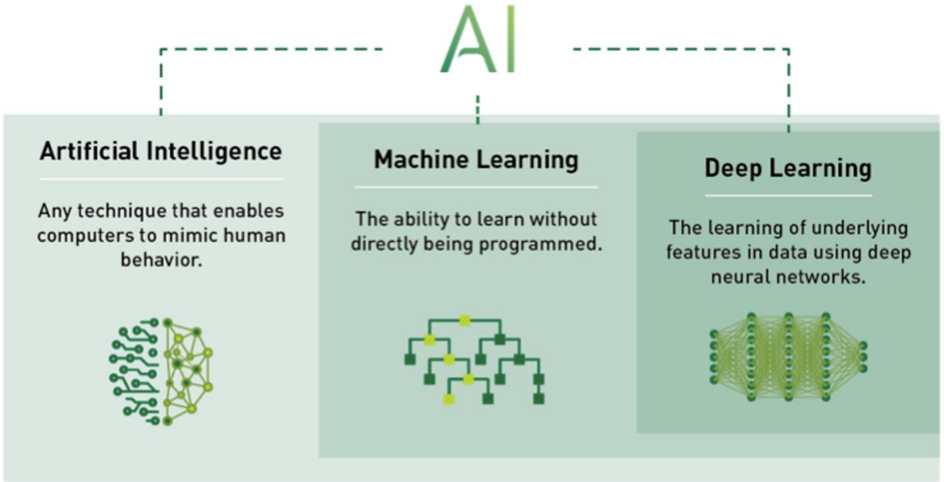
AI, ML & DL are areas in the process of **being explored** in view of the SOLEIL upgrade:

- **Experimental data processing**, to benefit from innovative data analytics and AI algorithms: to assess the data quality, cross-correlate current results with similar past experiments, obtain meta experiment results, …
  - SOLEIL member of **the LEAPS-INNOV** WP7 for data reduction and compression
  - SOLEIL member of the **BIG-MAP** project which intends to cohesively integrate machine learning, computer simulations and AI-orchestrated experiments and synthesis to accelerate battery materials discovery and optimization
- **Controls**: enhancement of the control of beam characteristics depending on a very large number of parameters, automatic detection of incidents and corrective – or even predictive – measures to be taken
- **Predictive maintenance** to optimize the availability of the infrastructures and ensure the expected safety level.
  - Considering solutions from digital industry initiatives that can help us manage the life cycle of our facilities.

From now on :

- **Transformation of the IT architecture** to accommodate the need to collect massive data to continuously train ML models.
- **Artificial intelligence**, **IoT** and **robotics** are topics in which SOLEIL trains or intends to train its staff.

# AI for Accelerators




**1/ automation and controls:** use of **on-line optimization algorithms** for exploring the phase space of parameters, defining new optimum working points for the accelerators, more robust settings to keep the same the performance irrespectively of the insertion device configuration.

**2/ beam diagnostics and data analysis:** Machine learning would be an added value for the operation of the beamlines and accelerators. In a control room, this could be a great help for the operator when confronted to a beam loss to quickly identify the cause of the incident. Connected with a **high-quality database**, **smart pattern matching** could be applied to identify source of beam losses

**3/ Predictive maintenance and anomaly detection could also strongly profit from AI and ML.**

The objectives would be to detect forthcoming incident, early deterioration of the accelerator performance.

Maintenance can be performed then either during machine day or shutdown period before any deterioration of the beam qualities. More other, upgrade leads to a significant increase of the amount of equipment to survey and maintain.

At SOLEIL, for example for the power supplies (factor x3), we will have to devise a new maintenance policy and to make **selective maintenance**. This is true for both hardware and software equipment and for control and accelerator components.

**4/ Simulation and optimization of the accelerators:** the aim is to have comprehensive models of the accelerators including **linear and nonlinear dynamics** using **MOGA, PSO**, etc. based algorithms, deep learning to optimize the performance.

Application of **neural networks in feedforward mode** have been demonstrated in ALS recently to correct the keep beam size variation below 0.6% RMS for STXM beamlines.

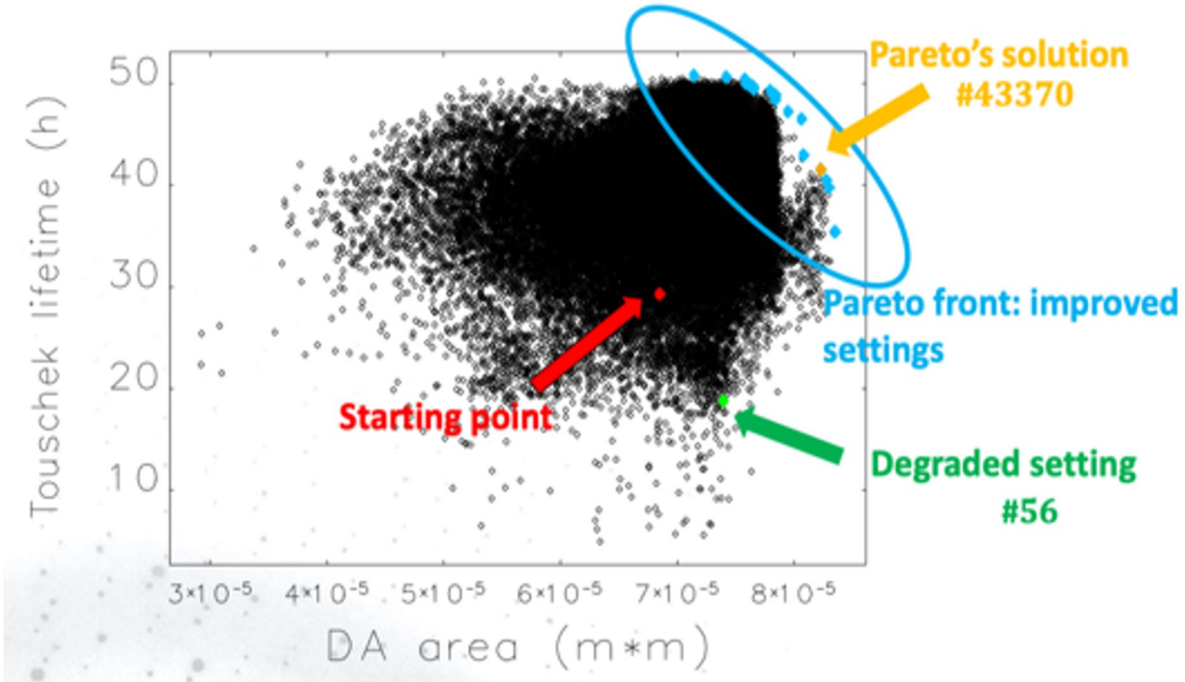
# Accelerator Beam Dynamics: simulation and online applications

- Performance optimization
  - Multi-objective Genetic Optimization (MOGA)
  - Particle Swarm Optimization (PSO)
  - Multi-Generation Gaussian Process Optimizer (MG-PGO)

Lifetime/injection efficiency improvement
Dynamic Aperture Momentum Aperture increase

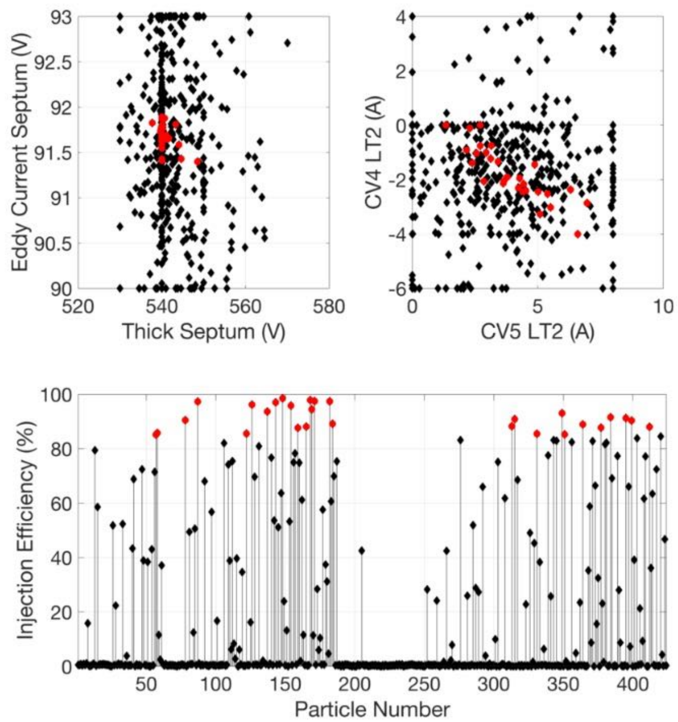
Xavier Nuel Gavaldà. Multi-Objective Genetic based Algorithms and Experimental Beam Lifetime Studies for the Synchrotron SOLEIL Storage Ring. Accelerator Physics [physics.acc-ph]. Université Paris-Saclay, 2016. English. ⟨NNT : 2016SACLS205⟩. ⟨tel-01385576⟩

The improvement of 50 % of the Touschek lifetime is confirmed by the experiments without jeopardizing the injection rate.

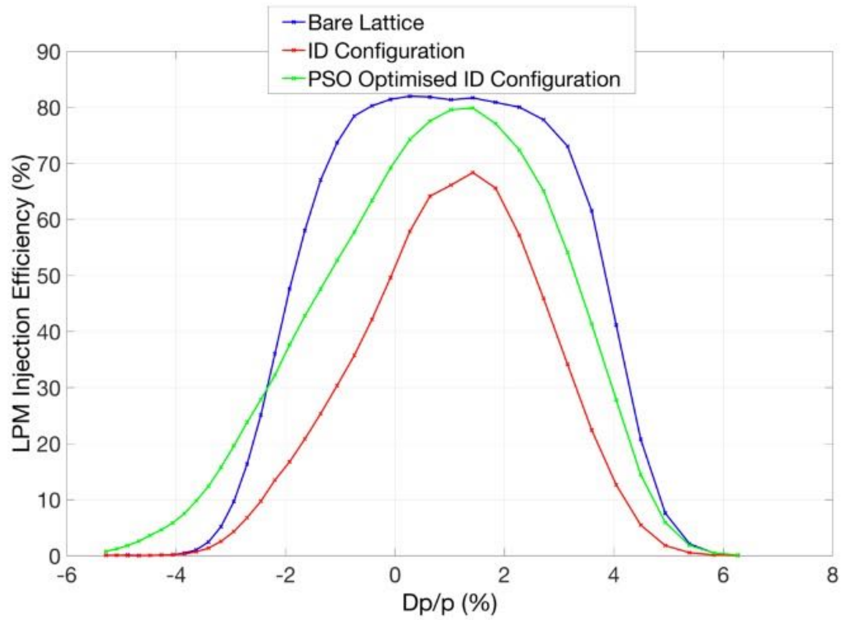


# AI to the service of Operation

## Online Particle Swarm Optimization



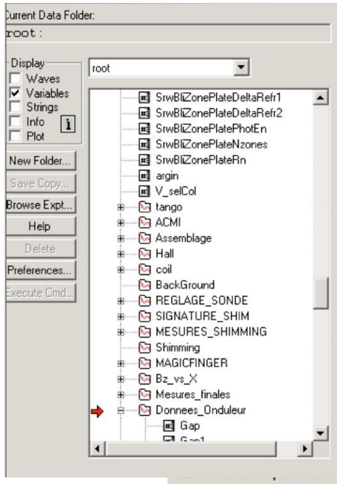

Automatic Injection Optimization in less Than 10 min



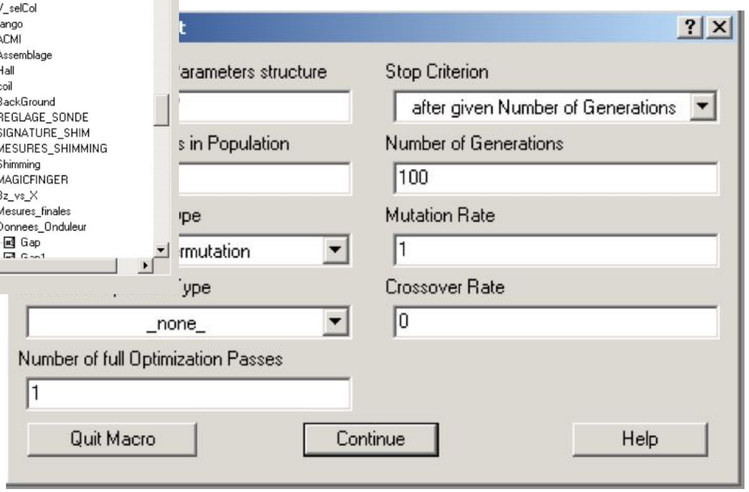

Energy Acceptance of the storage ring

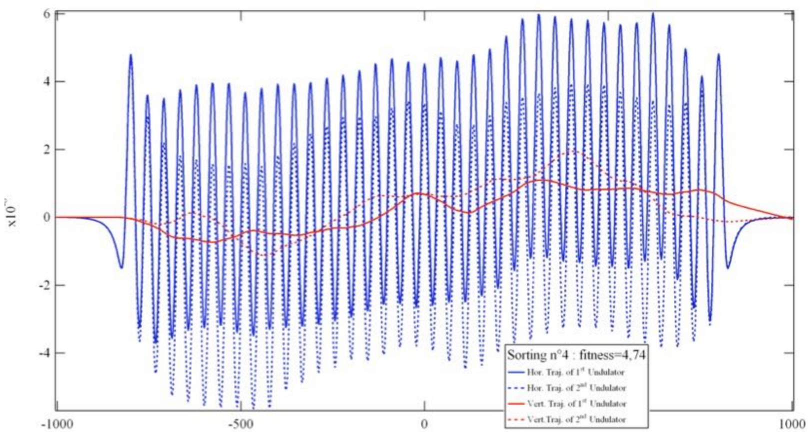
Aurelien Bence, Ji Li, Laurent Nadolski. First Application of Online Particle Swarm Optimization at SOLEIL. *10th International Particle Accelerator Conference*, May 2019, Melbourne, Australia. pp.MOPGW010, ⟨10.18429/JACoW-IPAC2019-MOPGW010⟩. ⟨hal-02222256⟩

# Undulator Construction




IDbuilder
Sorting, shimming, etc.




O. Chubar, O. Rudenko, C. Benabderrahmane, O. Marcouille, J. M. Filhol, *and* M. E. Couprie
"Application of Genetic Algorithms to Sorting, Swapping and Shimming of the SOLEIL Undulator Magnets", AIP Conference Proceedings 879, 359-362 (2007) https://doi.org/10.1063/1.2436074

# Application of DNN for feedback (LBNL/ALS)

New needs for SOLEIL

- Nanoscopium beamline
  - Low-photon flux experiment
  - Coherent sensitive experiment
- scanning transmission x-ray microscopy (STXM)

PHYSICAL REVIEW LETTERS **123,** 194801 (2019)

Featured in Physics

**Demonstration of Machine Learning-Based Model-Independent Stabilization of Source Properties in Synchrotron Light Sources**

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S. Liu†
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A. Hexemer, M. A. Marcus, C. N. Melton, H. Nishimura, and C. Sun
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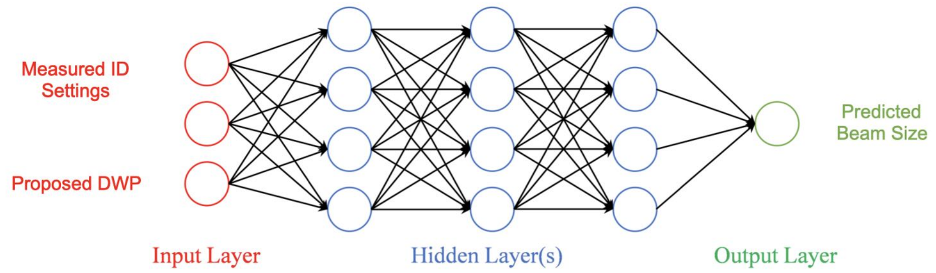
(Received 16 May 2019; revised manuscript received 23 August 2019; published 6 November 2019)

Synchrotron light sources, arguably among the most powerful tools of modern scientific discovery,

- Nonlinear optimization

## Neural Network — Used in Feed-Forward

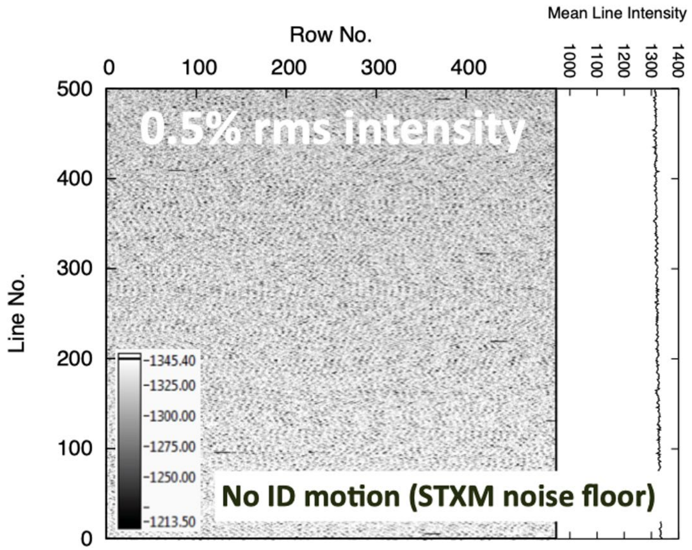
- Large parameters space (gap/phase) x tens of Ids freely control beam the beamlines



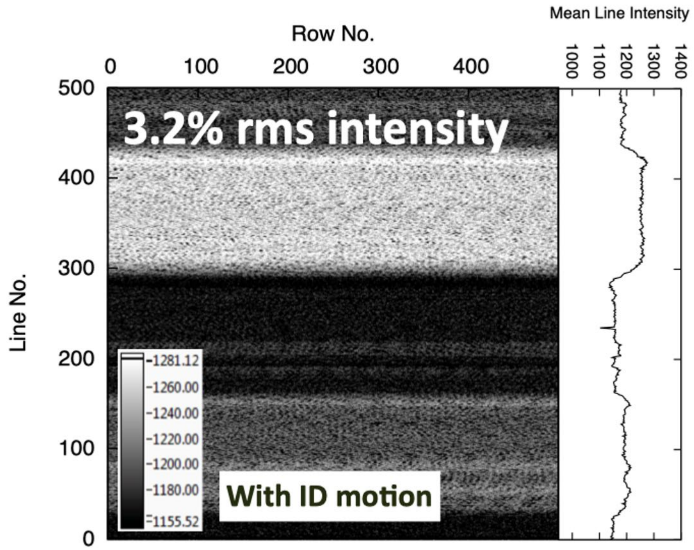

ALS Achievement: beamsize stabilization down to 0.2 µm (0.4% RMS) in daily operation

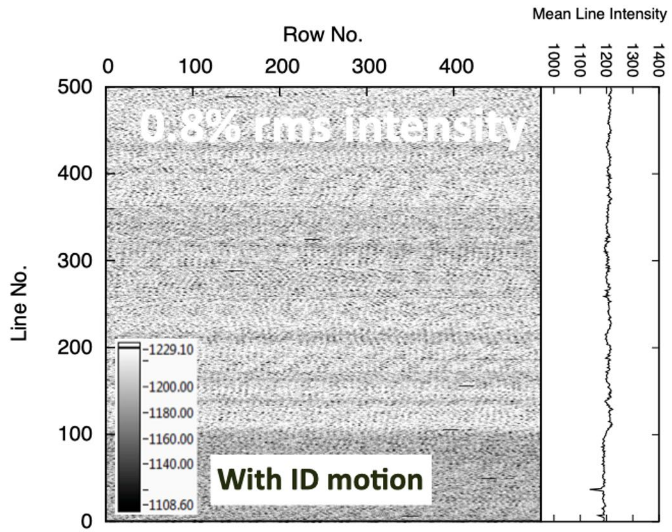
# NN-based FF Off vs. On at STXM Beamline 5.3.2.2

Scanning Transmission X-ray Microscopy



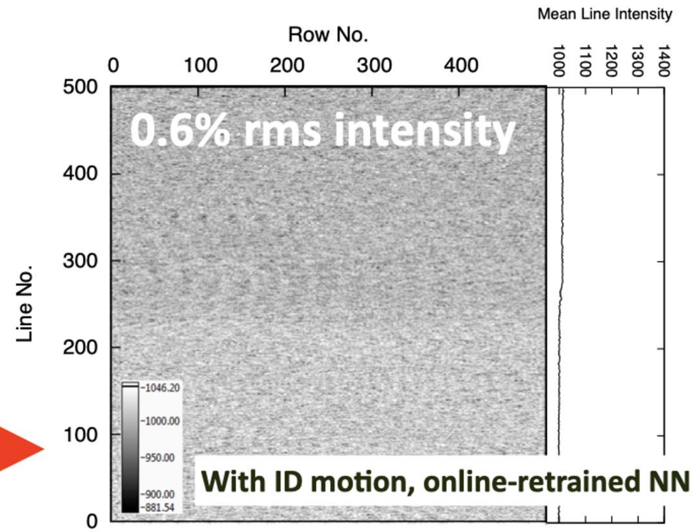

**NN-based FF off**



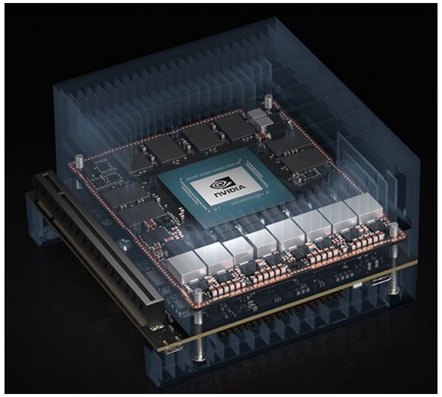




**NN-based FF on**

**Online Retraining**



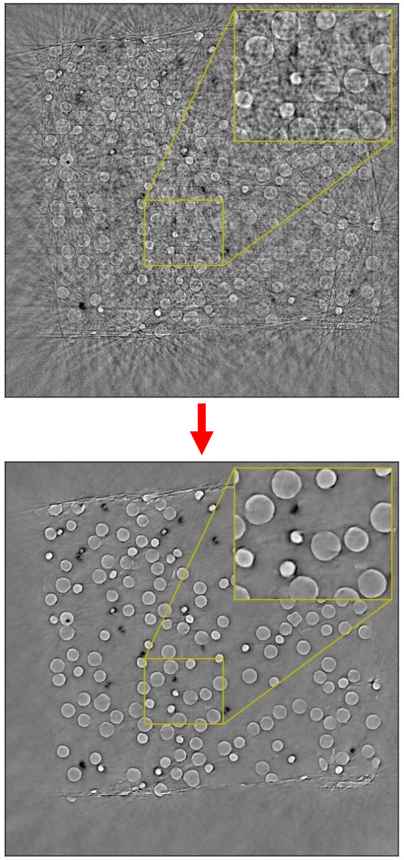
# AI machine learning (Data Treatment)



- Already apply **ML** (GA) on X-ray absorption (**XAS) data**.

- Experimenting **auto-processing right from the detector for image filtering**.

- **IA Deep Learning** on GPU **Jetson** Edge:
  - Beam auto-centring
  - Clean/filter images
  - Classify into categories (for inst. quality)
  - Tomography : Fast Reconstruction / filter



- Test: TomoGan, DragonFly, RootPainter…

- Applicable to: SAXS, MX, Diff, Imaging/tomo

# Digital Twins (Beam Line Simulation)

We provide **on-demand data treatment** environments (virtual machines) including beamline simulation tools.

**McXtrace** <http://www.mcxtrace.org> with interfaces to

- Spectra, Simplex, Genesis13
- Shadow/OASYS
- GEANT4, PHITS

McXtrace allows to describe a BL as :

- **photon source → optics → samples → detectors**

The samples can be:

- powders, SX, SAXS, absorption, ...

McXtrace may optimize beamline parameters for flux/resolution, and runs on HPC/GPU.

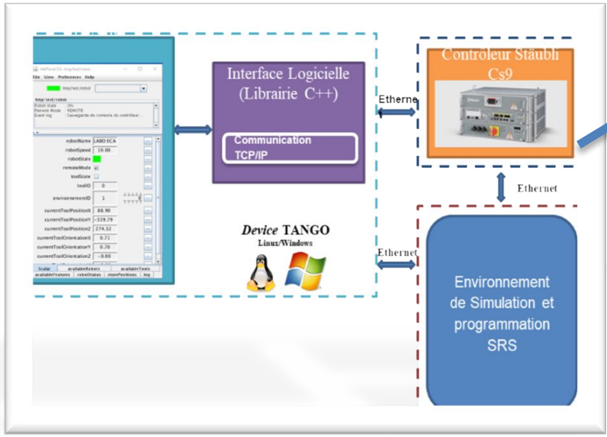
# Digital Twinning for Mechatronics Apps

- Robotics :

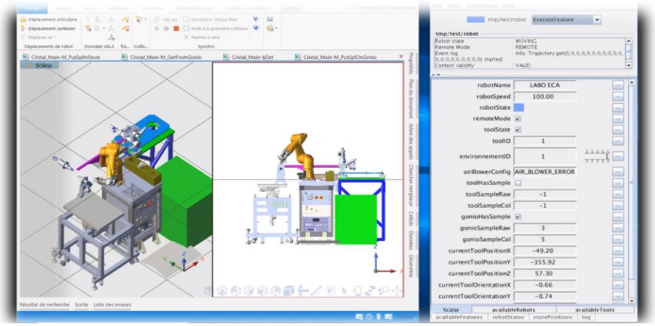
CRISTAL BeamLine:
Pick-and-place

*position sample holders from their rack to the BL diffractometer, then return them to the rack after analysis*

Control system




At the BeamLine : https://youtu.be/MbFGQdI-D24



Simulation: https://youtu.be/HMeN9lsH9xI

*Switching control system of a robotic application **from** simulation on a robotic cell "Model" **to** the beamline hutch. This approach allow **simulating trajectories and off-line** robot programs and **validating mechanical integration** with all its elements from 3D-CAD before its operation in the real world.*

- Predictive anti-collision

*Definition and Validation **anticollision "Model"** prior to its implementation in the control of the mechatronic system in the near experimental environment.*

3D Model

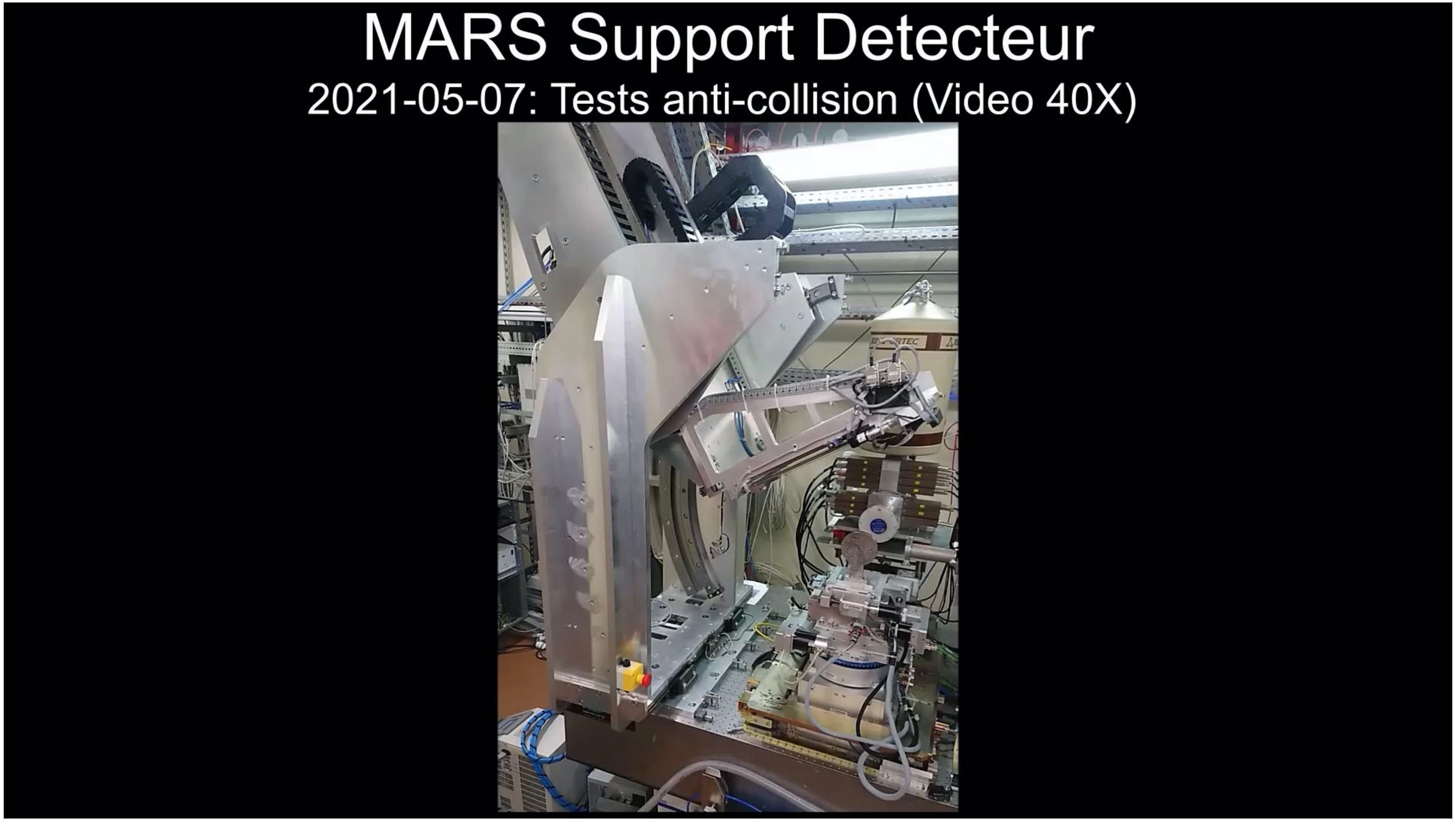
Simulation

Set of equations

Motion Controller

MARS BeamLine: 2D-detector holder

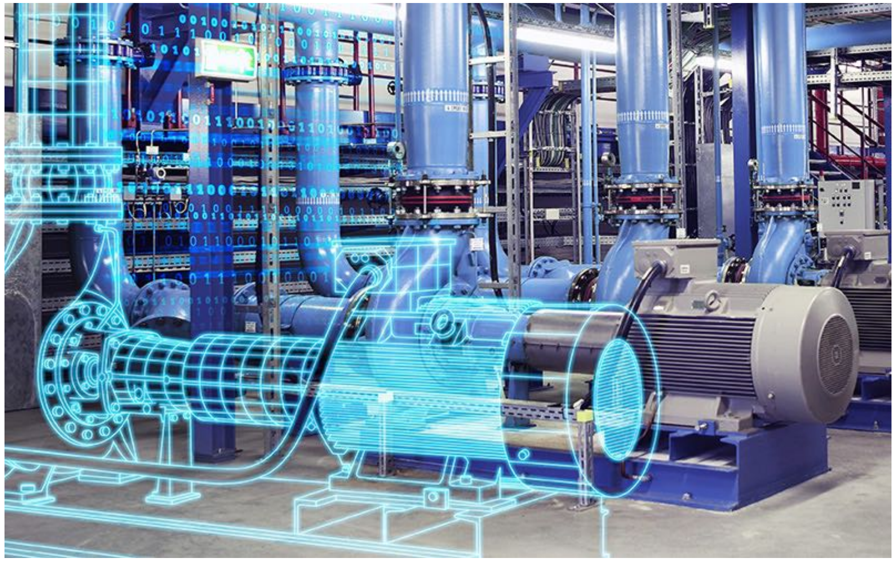
# Anticollision System and Digital Twin



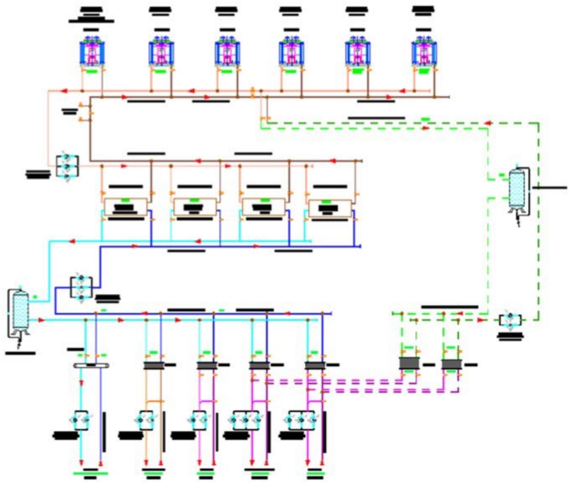
# Digital Twin for the Utility Station

## New Station project (2021-2024): national French recovery plan)

- Pre-commissioning the new Utility Station
- Optimization of the process
- Preparing maintenance
- Testing software upgrade
- Testing hardware upgrade
- Training of the technical staff



Station projetée



# On the Detectors side

## ❑ LEAPS Integrated Platform

- Digital Twin
- Machine Learning
- Virtual Diagnostic
- Androids for Remote Access
- **Design for a Fully Automated User Beamline (ABL)**

SOLEIL Detectors group possible implication
*(in discussion)*

Objective: this 'project' aims to study how an ideal, self-aligning and self-calibrating beamline could look like!

*First meeting with other synchrotrons detectors groups (LEAPS partners of WG1.1) → November 2020*

Main questions raised during this first meeting:

- When do we lose beamtime and why / how can it be improved?
- Automatic data taking and analysis?
- Which diagnostics on the X-ray beam path? Auto-calibration of detectors? etc

→ A universal solution is certainly not possible (various BLs and experimental techniques, and not always repetitive)

*This topic is very large and covers detectors domain, but not only: also optics, sample environment, etc. Experimenters should be also in the loop*

# On the Detectors Side

- <u>Two areas in discussion:</u>

  1. Automatic setup of all components after changing a parameter (eg wavelength or beam size), and automatic periodic realignment to correct drifts
  2. Automatic data taking, data analysis and steering of data taking campaign (works for certain measurements, not for many experiments)

- <u>Proposed work-packages</u>

✓ **Automation and fault tolerance of repetitive tasks**: beamline alignment, focus optimization…

✓ **Automatic detector calibration**, software configuration, parameter selection

✓ **Sample tracking, loading, changing**

✓ **Remote experimenter in the loop**: remote data analysis, experiment feedback, remote presence

✓ **Beyond remote desktop**: Improving beamline control interfaces for remote presence

➡ ***Kick-off the project with a preliminary phase*** *in which the technical and scientific staff at facilities should be contacted and surveyed to define* ***the different needs and objectives***

# Thank you for your attention
# Questions ?

## Acknowledgments


- Direction: B. Gagey, A. Nadji
- Y.-M. Abiven (Electronics for Control Acquisition)
- E. Farhi (GRADES group)
- F. Orsini (Detector group)
- Accelerators Physics Group

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