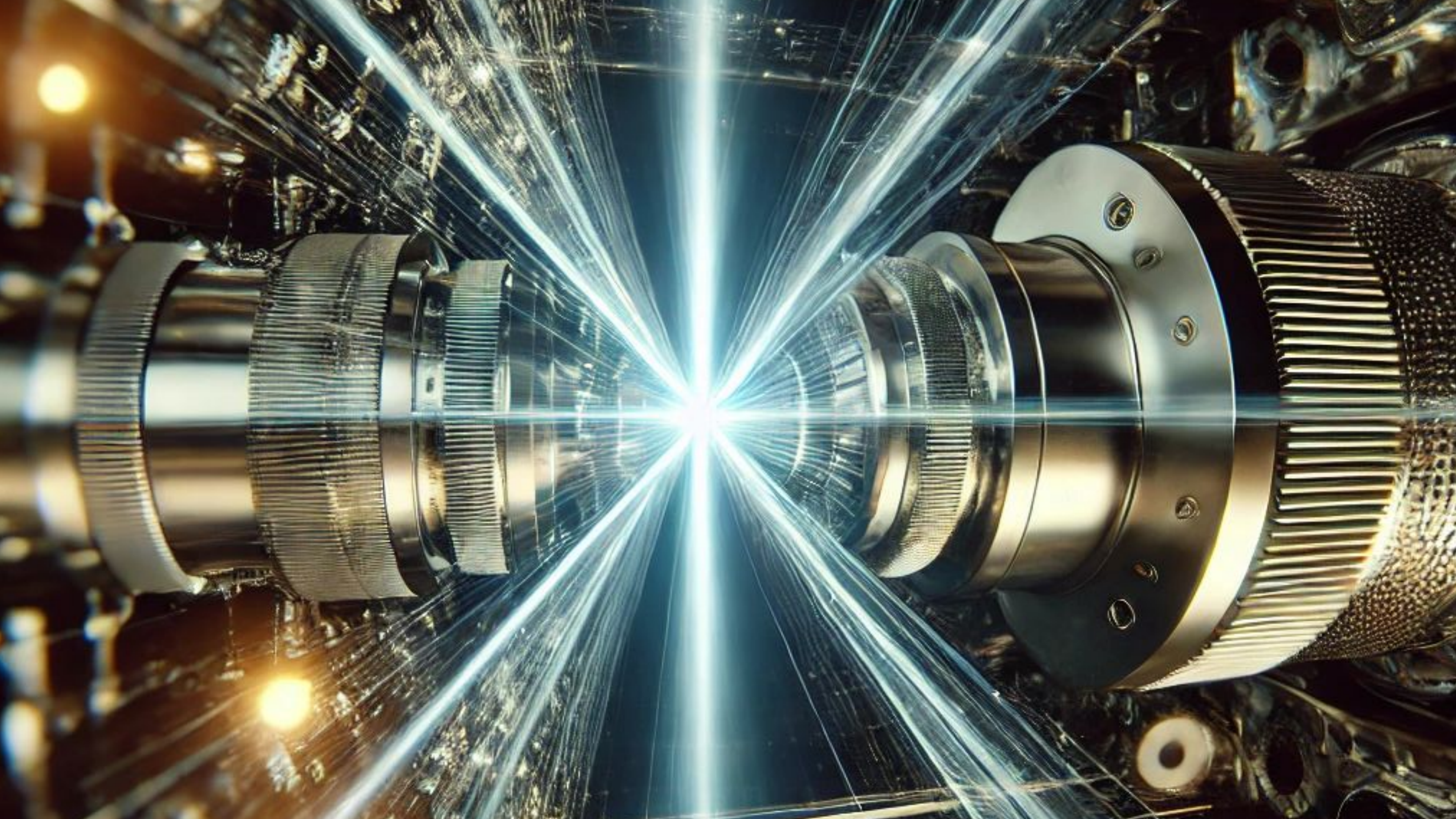
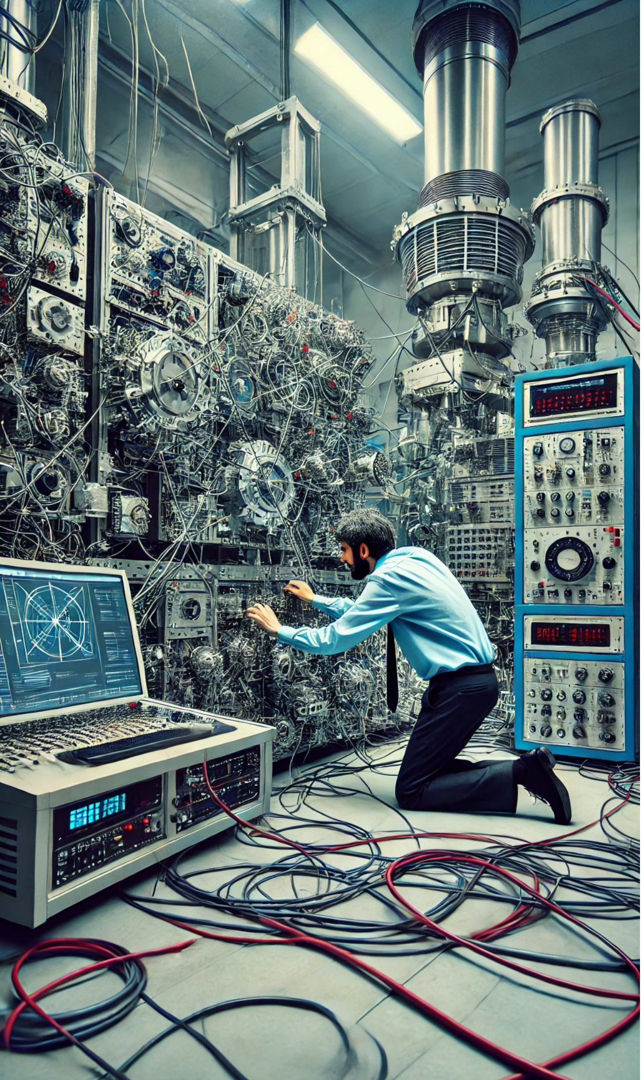
# PROPOSTA DI GRANT GIOVANI IN CSN5 ANNO 2024

# OPTIMAL

**Simone Manti**

Frascati, 09/07/2024





# Challenges in X-ray Beamline Optimization

Manual Optimization of Parameters

Dependence on human input

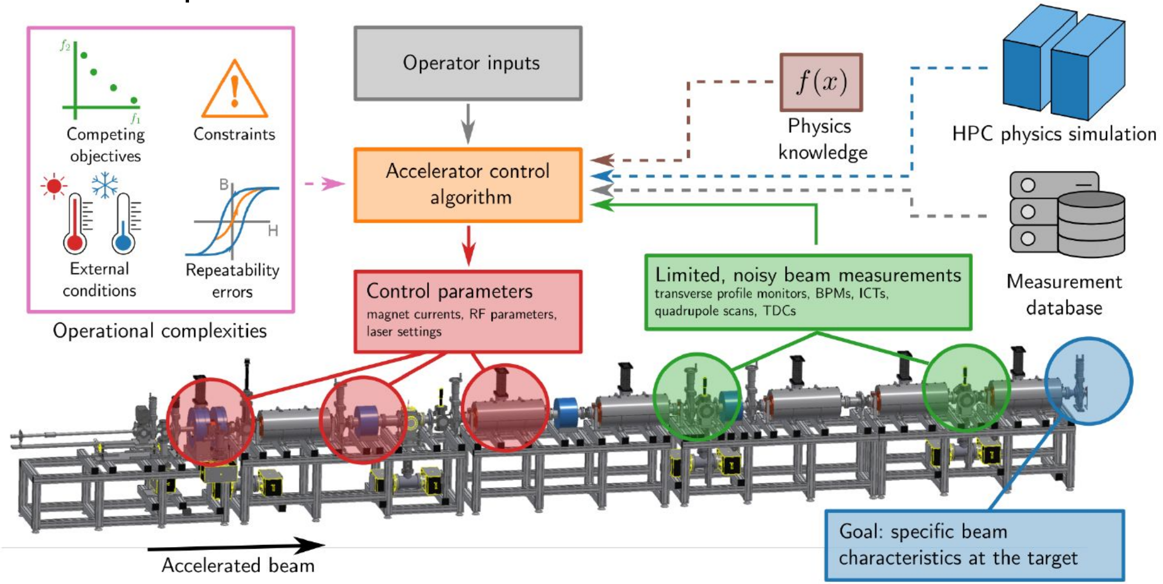
Challenges in reproducibility

Time constraints

# State of the Art

**Advancements:**

- **Machine Learning** algorithms can learn from data to identify optimal settings.
- **Bayesian Optimization (BO)** utilizes surrogate models (Gaussian Processes) to guide optimization, effective for problems with noisy and time-consuming acquisition functions.
- **Reinforcement Learning (RL)** builds a model through iterative feedback suitable for scenarios requiring large numbers of control parameters.




Roussel, Ryan, et al. "Bayesian optimization algorithms for accelerator physics." Phys. Rev. Accel. Beams (2024).

# State of the Art

**Advancements:**

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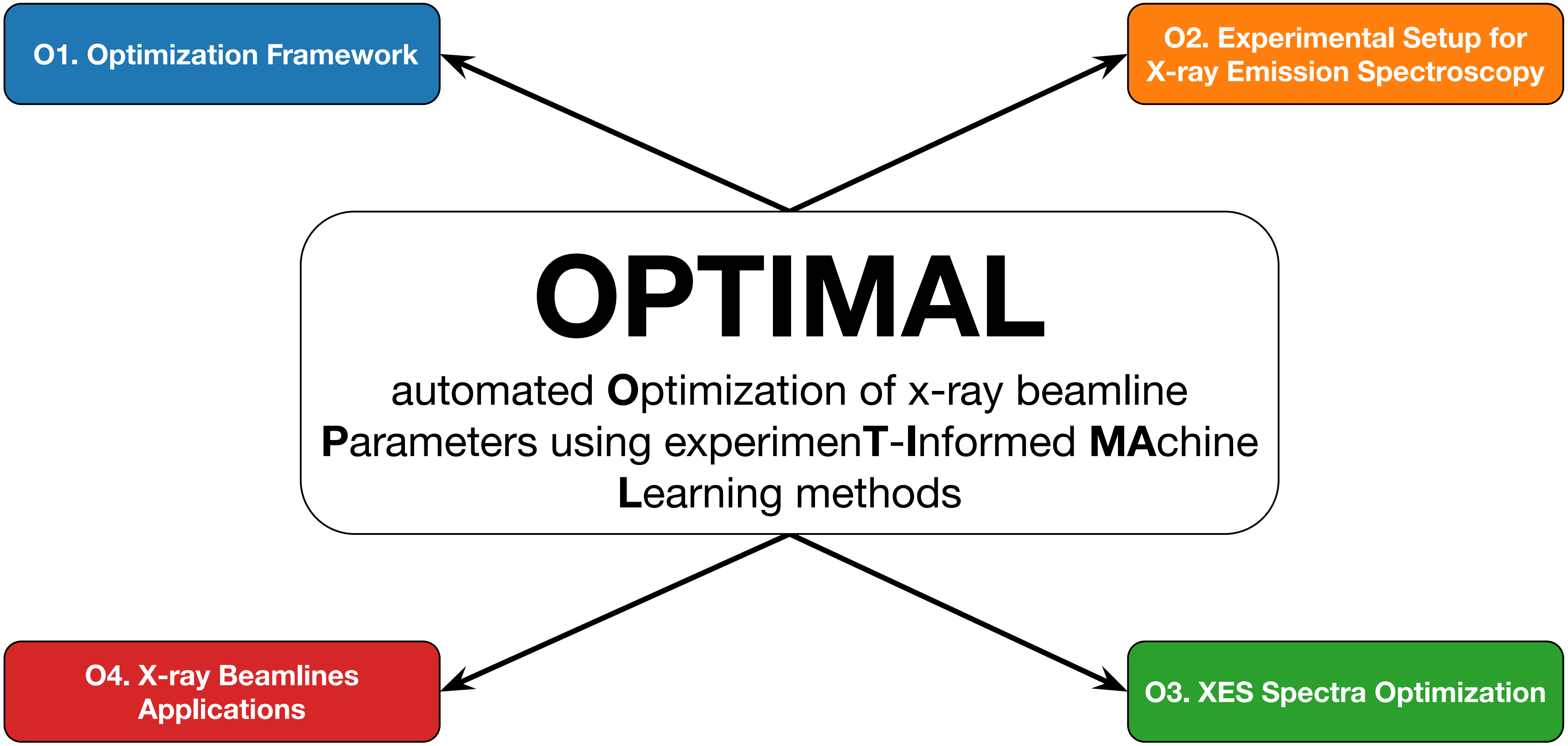
**Applications:**

- BO and RL have been successfully applied in various domains, including particle accelerators, detector designs, and laser pulse optimization in Free-Electron Lasers.
- **X-ray Beamlines:**
  - Optimize parameters for X-ray Absorption Spectroscopy
  - Autoalignment of a X-ray focusing system

**Current Gaps:**

- Fewer applications of BO in X-ray beamlines compared to other areas.
- Opportunity to develop ML-aided techniques to enhance efficiency and in X-ray experiments.


O1. Optimization Framework
O2. Experimental Setup for X-ray Emission Spectroscopy
OPTIMAL
automated **O**ptimization of x-ray beamline **P**arameters using experimen**T**-**I**nformed **MA**chine **L**earning methods
O4. X-ray Beamlines Applications
O3. XES Spectra Optimization

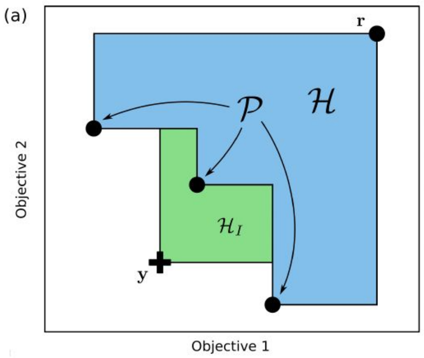
# O1. Optimization Framework

Framework for optimizing experiments based on X-ray detection

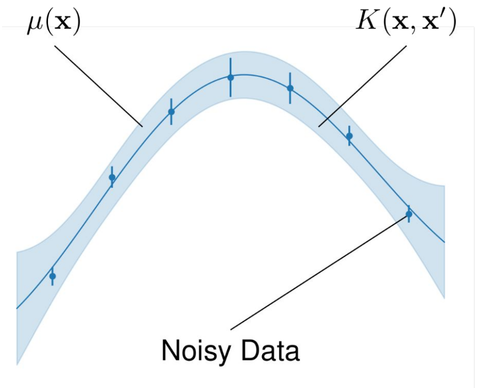
Modules for Data Acquisition, Setup Control, Simulations, and **Multi-Objective Optimization**

Two techniques: **Bayesian Optimization** and **Reinforcement Learning**

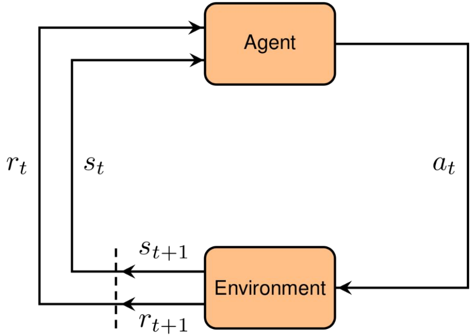
Employ **Machine Learning** models trained on **Ray-Tracing simulations** of the experiment




Pareto Front



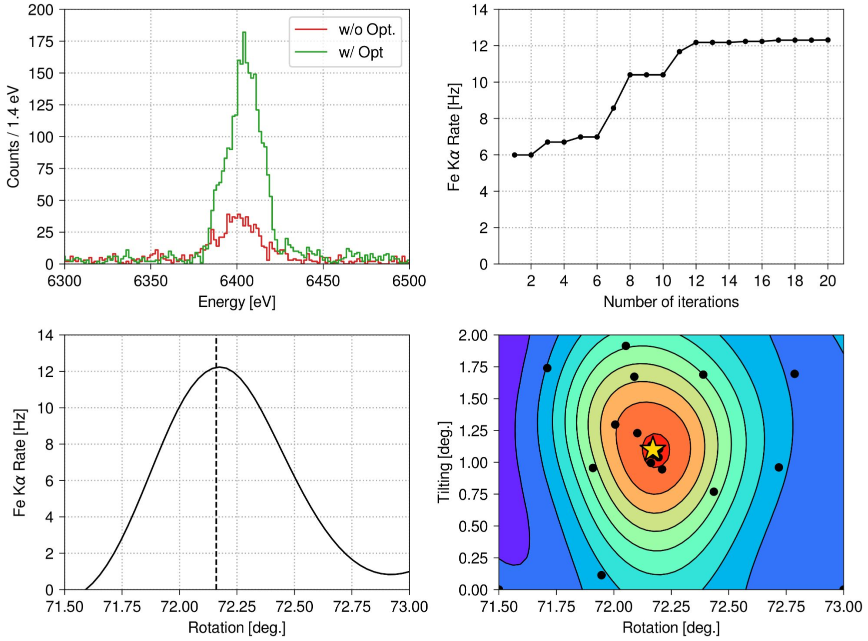

Bayesian Optimization

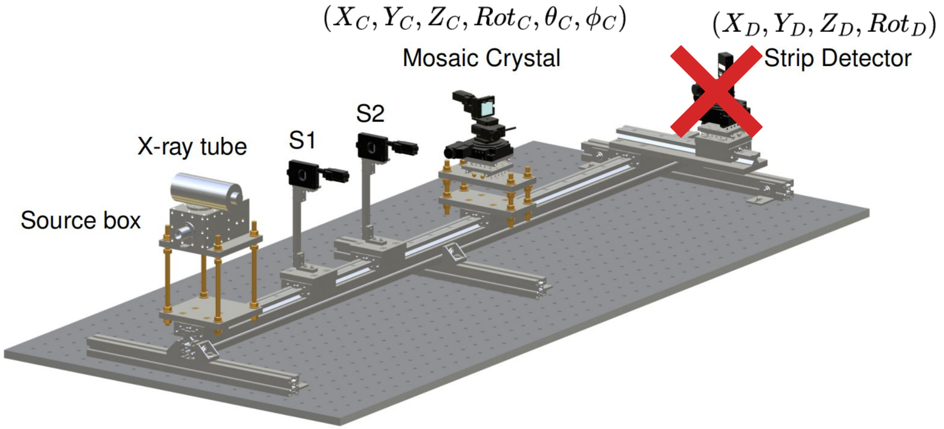



Reinforcement Learning

# O2. Experimental Setup for X-ray Emission Spectroscopy (XES)

I performed **feasibility test** at the LNF studying FeK$\alpha$ emission line, have shown that optimizing parameters for XES, can lead to a significant improvement of the emission line's rate under study, with a gain of a **factor 10** in the **overall acquisition time**



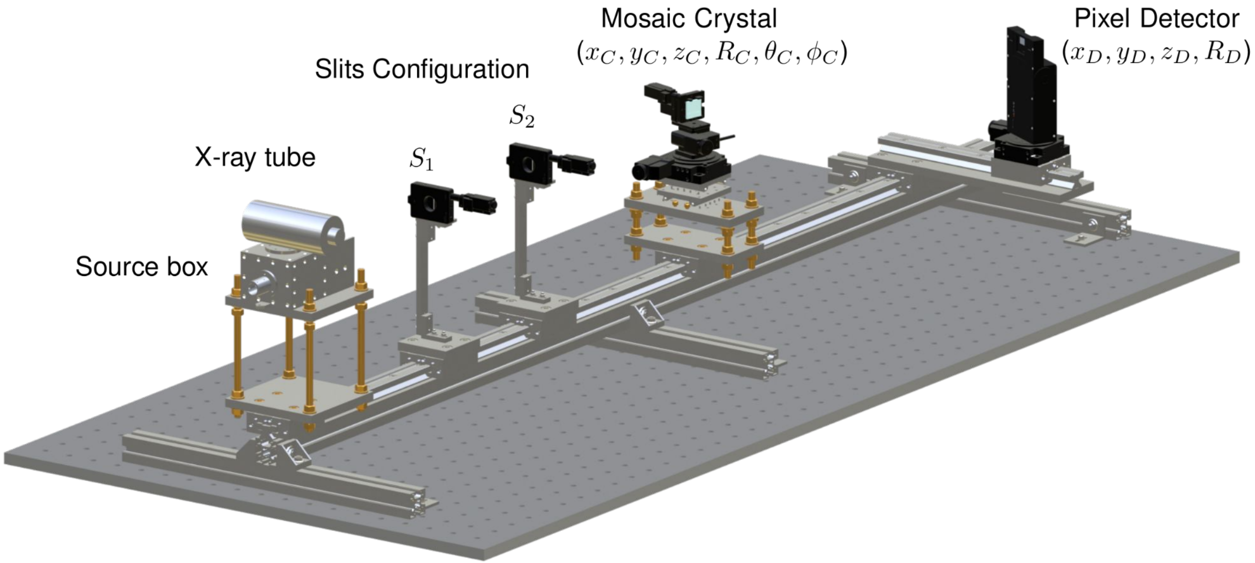

The current VOXES setup is inadequate for this purpose, as a **Strip Detector** with 1D spectra data limits the effectiveness of ML features extraction for the optimization loop!

# O2. Experimental Setup for XES

A pixel detector with a **2D spectrum** offers significantly more information, enhancing the training phase, and thus the spectral feature extraction part

The best balance solution between cost and project requirements is the **AdvaPIX Timepix3** from **ADVACAM** (Prague, Czech Republic).

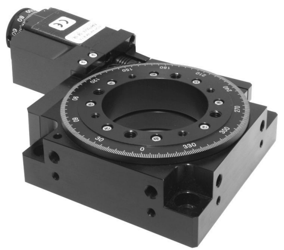
Plus a **4-axis motorized stage** system from **STANDA** company, like the old ones, for their easy communication interface with the framework using the **libximc package.**



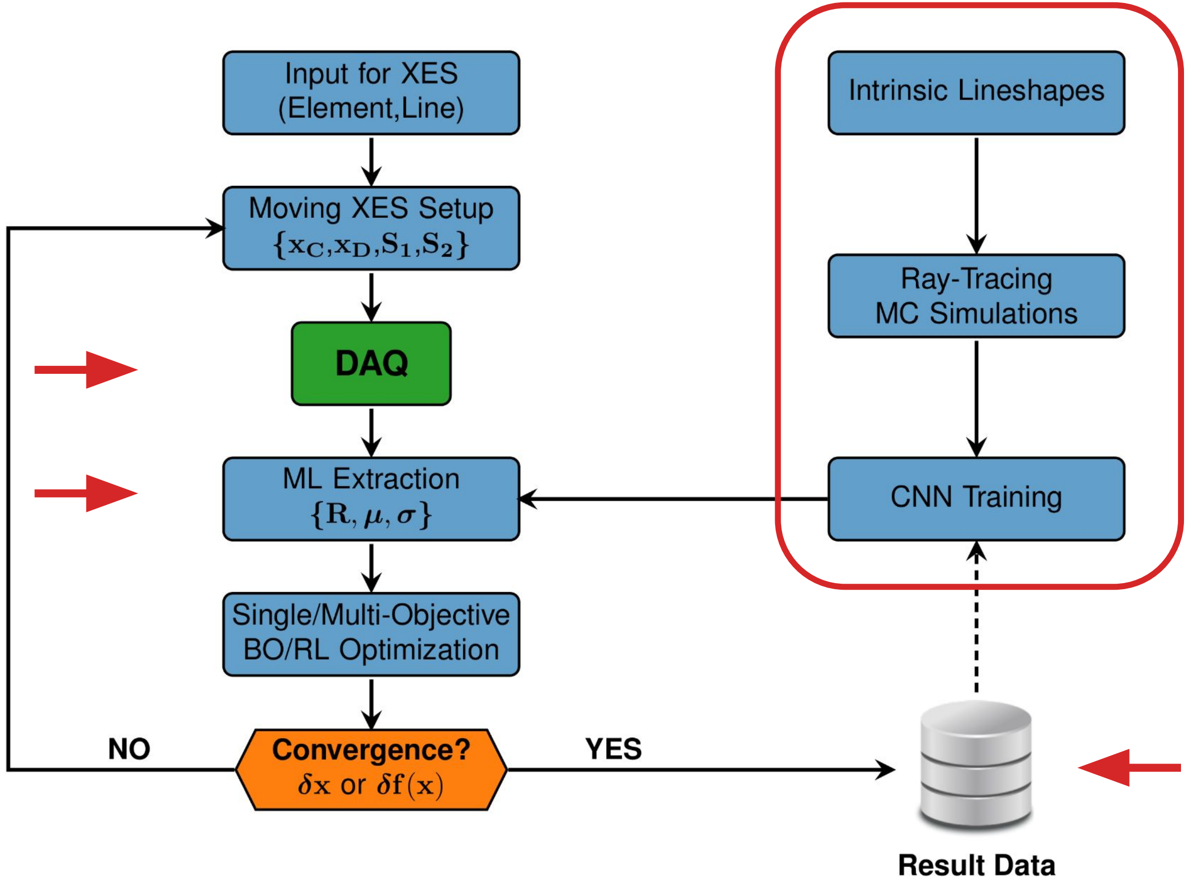

**AdvaPIX Timepix3**

- Energy range of 5.4 to 20 keV
- Si sensor thickness of 300 µm
- Pixel size of 55 µm
- Resolution 512×256 pixels
- Sensitive Area 14x14 mm

**STANDA motorized stage**



# O3. Spectra Optimization Workflow





Kristian Piscicchia, Sandro Donadi, **Simone Manti**, Angelo Bassi, Maanel Derakhshani, Lajos Diósi, Catalina Curceanu, "*X-Ray Emission from Atomic Systems Can Distinguish between Prevailing Dynamical Wave-Function Collapse Models.*" *Physical Review Letters* 132.25 (2024): 250203.

**Simone Manti**, Fabrizio Napolitano, Alberto Clozza, Catalina Curceanu, Gabriel Moskal, Kristian Piscicchia, Diana Sirghi and Alessandro Scordo. "*Enhancing Performances of the VOXES Bragg Spectrometer for XES Investigations.*" *Condensed Matter* 9.1 (2024): 19.

**Simone Manti**, Mark Kamper Svendsen, Nikolaj R. Knøsgaard, Peder M. Lyngby & Kristian S. Thygesen, "*Exploring and Machine Learning structural instabilities in 2D materials.*" *npj Computational Materials* 9.1 (2023): 33.

**Simone Manti**, Fabian Bertoldo, Sajid Ali & Kristian S. Thygesen, "*Quantum point defects in 2D materials-the QPOD Database.*" *npj Computational Materials* 8.1 (2022): 56.

# O4. X-ray Beamlines Applications

**Goal:**

- Test the possibility of applying the developed optimization framework to the **DAFNE-Light** beam facility at LNF.

**Expected Outcomes:**

- **Demonstrate Framework's Potential:** Showcase the adaptability of the framework to any X-ray beamline.

- **Identify Applications:** Document potential applications or experiments that can benefit from these enhancements, both within LNF and externally.

# Organization

**WP1 - Developing the Optimization Framework (Months 1-12)**

- D1.1 Technical note on the optimization framework (Month 6)
- D1.2 Documentation on raytracing simulations (Month 6)
- D1.3 Summary of training and validation of ML models (Month 6):
- M1 Framework implemented (Month 12).

**WP2 - Assembling the experimental setup (Months 1-15)**

- D2.1 Report on the integration of detector (Month 6)
- D2.2 Summary on measurements with the new detector (Month 12)
- M2 Detector integrated (Month 6)

**WP3 - Optimization of XES measurement (Months 13-24)**

- D3.1 Results of optimization with the new setup (Month 21)

**WP4 - Dissemination and Validation of results (Months 19-24)**

- M3 Measurement at DAFNE-Light (Month 21)

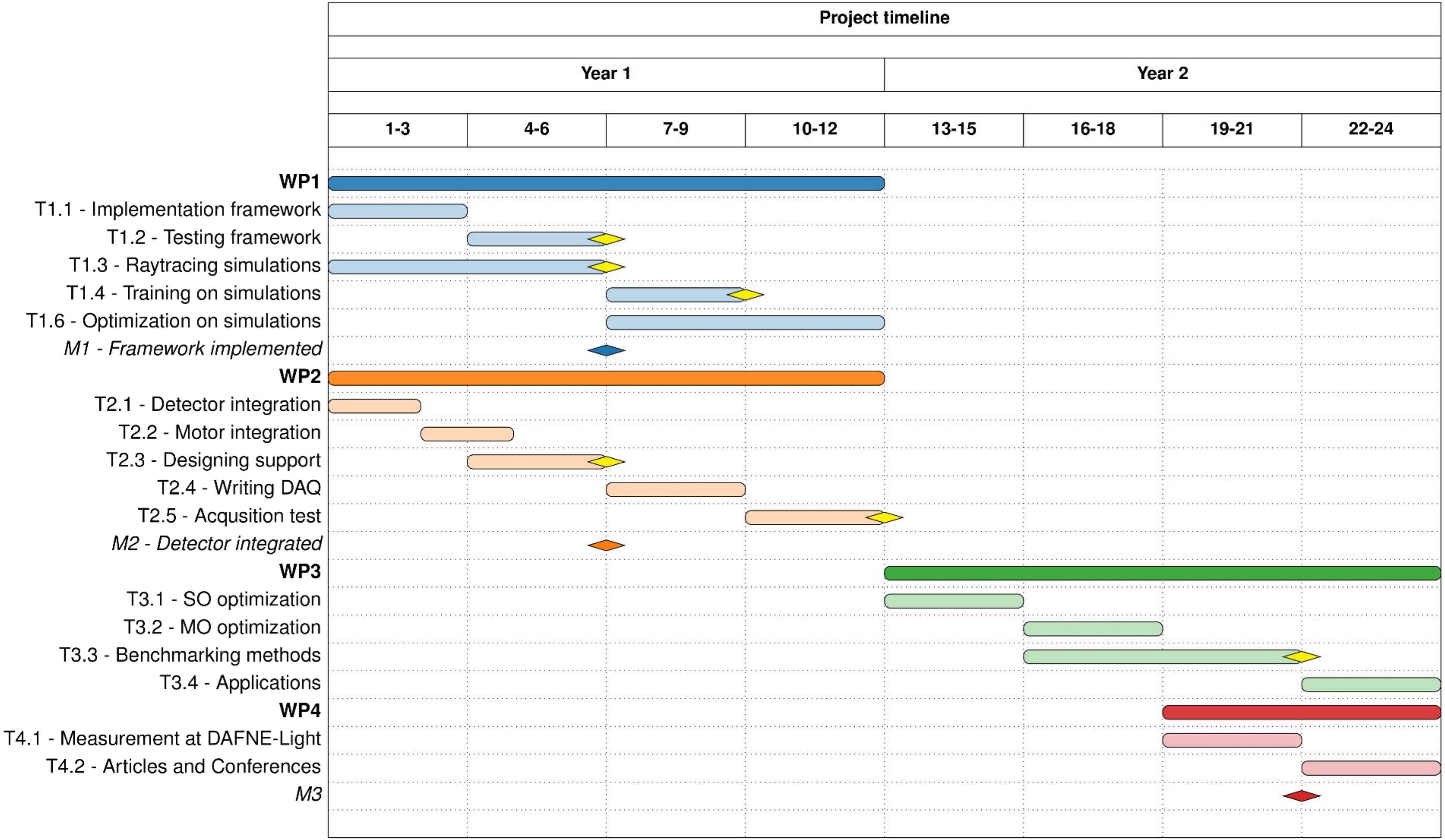
**Simone Manti** (INFN,LNF)
FTE:1.0 All WPs

**Alberto Clozza** (INFN,LNF)
FTE:0.3 WP2

**Alessandro Scordo** (INFN,LNF)
FTE:0.3 WP1,WP3

**Massimiliano Bazzi** (INFN,LNF)
FTE:0.1 WP2

**Catalina Curceanu** (INFN,LNF)
FTE:0.1 WP4



Project timeline
Year 1
Year 2
1-3
4-6
7-9
10-12
13-15
16-18
19-21
22-24
WP1
T1.1 - Implementation framework
T1.2 - Testing framework
T1.3 - Raytracing simulations
T1.4 - Training on simulations
T1.6 - Optimization on simulations
M1 - Framework implemented
WP2
T2.1 - Detector integration
T2.2 - Motor integration
T2.3 - Designing support
T2.4 - Writing DAQ
T2.5 - Acqusition test
M2 - Detector integrated
WP3
T3.1 - SO optimization
T3.2 - MO optimization
T3.3 - Benchmarking methods
T3.4 - Applications
WP4
T4.1 - Measurement at DAFNE-Light
T4.2 - Articles and Conferences
M3

# Synergies

## INFN Scientific Commissions and Collaborations:

- **VOXES** (LNF)
- **DAFNE-Light** (LNF)
- **EuAPS** (LNF)
- **EuPRAXIA** (LNF)

- **SPHINX** (CSN5)

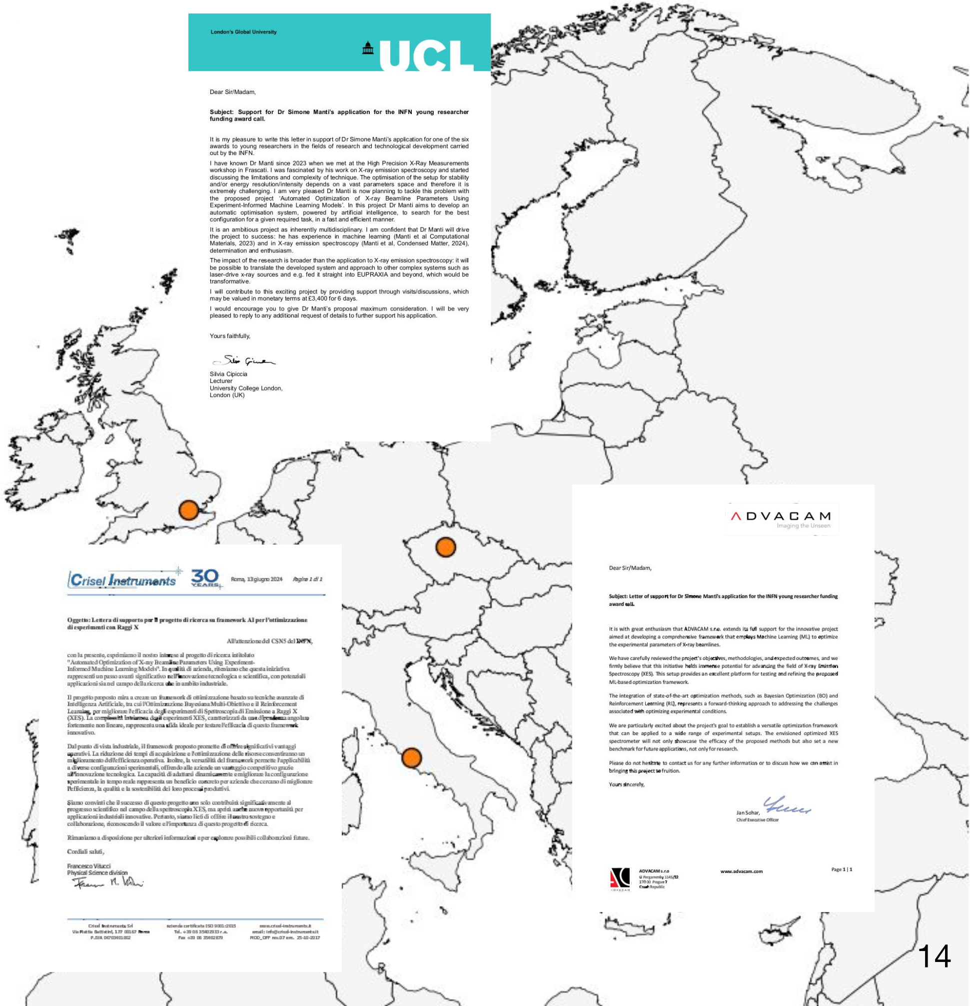
## National and International Research Institutions:

- **Advanced X-Ray Imaging Group** (London)

## Industry and Private Sector

- **ADVACAM** (Prague)

- **CRISEL** (Rome)



London's Global University

UCL

Dear Sir/Madam,

**Subject: Support for Dr Simone Manti's application for the INFN young researcher funding award call.**

It is my pleasure to write this letter in support of Dr Simone Manti's application for one of the six awards to young researchers in the fields of research and technological development carried out by the INFN.

I have known Dr Manti since 2023 when we met at the High Precision X-Ray Measurements workshop in Frascati. I was fascinated by his work on X-ray emission spectroscopy and started discussing the limitations and complexity of technique. The optimisation of the setup for stability and/or energy resolution/intensity depends on a vast parameters space and therefore it is extremely challenging. I am very pleased Dr Manti is now planning to tackle this problem with the proposed project 'Automated Optimization of X-ray Beamline Parameters Using Experiment-Informed Machine Learning Models'. In this project Dr Manti aims to develop an automatic optimisation system, powered by artificial intelligence, to search for the best configuration for a given required task, in a fast and efficient manner.

It is an ambitious project as inherently multidisciplinary. I am confident that Dr Manti will drive the project to success: he has experience in machine learning (Manti et al Computational Materials, 2023) and in X-ray emission spectroscopy (Manti et al, Condensed Matter, 2024), determination and enthusiasm.

The impact of the research is broader than the application to X-ray emission spectroscopy: it will be possible to translate the developed system and approach to other complex systems such as laser-drive x-ray sources and e.g. fed it straight into EUPRAXIA and beyond, which would be transformative.

I will contribute to this exciting project by providing support through visits/discussions, which may be valued in monetary terms at £3,400 for 6 days.

I would encourage you to give Dr Manti's proposal maximum consideration. I will be very pleased to reply to any additional request of details to further support his application.

Yours faithfully,

Silvia Cipiccia
Lecturer
University College London,
London (UK)

Crisel Instruments 30 YEARS Roma, 13 giugno 2024 Pagina 1 di 1

**Oggetto: Lettera di supporto per il progetto di ricerca su framework AI per l'ottimizzazione di esperimenti con Raggi X**

All'attenzione del CSN5 del INFN,

con la presente, esprimiamo il nostro interesse al progetto di ricerca intitolato "Automated Optimization of X-ray Beamline Parameters Using Experiment-Informed Machine Learning Models". In qualità di azienda, riteniamo che questa iniziativa rappresenti un passo avanti significativo nell'innovazione tecnologica e scientifica, con potenziali applicazioni sia nel campo della ricerca che in ambito industriale.

Il progetto proposto mira a creare un framework di ottimizzazione basato su tecniche avanzate di Intelligenza Artificiale, tra cui l'Ottimizzazione Bayesiana Multi-Obiettivo e il Reinforcement Learning, per migliorare l'efficacia degli esperimenti di Spettroscopia di Emissione a Raggi X (XES). La complessità intrinseca degli esperimenti XES, caratterizzati da una dipendenza angolare fortemente non lineare, rappresenta una sfida ideale per testare l'efficacia di questo framework innovativo.

Dal punto di vista industriale, il framework proposto promette di offrire significativi vantaggi operativi. La riduzione dei tempi di acquisizione e l'ottimizzazione delle risorse consentiranno un miglioramento dell'efficienza operativa. Inoltre, la versatilità del framework permette l'applicabilità a diverse configurazioni sperimentali, offrendo alle aziende un vantaggio competitivo grazie all'innovazione tecnologica. La capacità di adattarsi dinamicamente e migliorare la configurazione sperimentale in tempo reale rappresenta un beneficio concreto per aziende che cercano di migliorare l'efficienza, la qualità e la sostenibilità dei loro processi produttivi.

Siamo convinti che il successo di questo progetto non solo contribuirà significativamente al progresso scientifico nel campo della spettroscopia XES, ma aprirà anche nuove opportunità per applicazioni industriali innovative. Pertanto, siamo lieti di offrire il nostro sostegno e collaborazione, riconoscendo il valore e l'importanza di questo progetto di ricerca.

Rimaniamo a disposizione per ulteriori informazioni e per esplorare possibili collaborazioni future.

Cordiali saluti,

Francesco Vitucci
Physical Science division

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ADVACAM
Imaging the Unseen

Dear Sir/Madam,

**Subject: Letter of support for Dr Simone Manti's application for the INFN young researcher funding award call.**

It is with great enthusiasm that ADVACAM s.r.o. extends its full support for the innovative project aimed at developing a comprehensive framework that employs Machine Learning (ML) to optimize the experimental parameters of X-ray beamlines.

We have carefully reviewed the project's objectives, methodologies, and expected outcomes, and we firmly believe that this initiative holds immense potential for advancing the field of X-ray Emission Spectroscopy (XES). This setup provides an excellent platform for testing and refining the proposed ML-based optimization framework.

The integration of state-of-the-art optimization methods, such as Bayesian Optimization (BO) and Reinforcement Learning (RL), represents a forward-thinking approach to addressing the challenges associated with optimizing experimental conditions.

We are particularly excited about the project's goal to establish a versatile optimization framework that can be applied to a wide range of experimental setups. The envisioned optimized XES spectrometer will not only showcase the efficacy of the proposed methods but also set a new benchmark for future applications, not only for research.

Please do not hesitate to contact us for any further information or to discuss how we can assist in bringing this project to fruition.

Yours sincerely,

Jan Sohar,
Chief Executive Officer

ADVACAM s.r.o
U Pergamenky 1145/12
170 00 Prague 7
Czech Republic

www.advacam.com

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# Cost

The overall cost of **OPTIMAL** is **230 k€**, of which **124 k€** are in-kind contributions, and **106 k€** are requested for the project: **70 k€** for the first year and **36 k€** for the second year of the project.

| Year | Activity | Cost (€) | In-Kind Cost (€) |
|---|---|---|---|
| Year 1 | XES setup | 0 | 120000 |
| Year 1 | Pixel Detector | 50000 | 0 |
| Year 1 | Motors | 10000 | 0 |
| Year 1 | Support | 3000 | 0 |
| Year 1 | Workstation + GPU | 7000 | 0 |
| Year 2 | Jetson Xavier GPU | 3000 | 0 |
| Year 2 | Travel to AXIm | 0 | 4000 |
| Year 2 | Target elements | 2000 | 0 |
| Year 2 | Publications | 3000 | 0 |
| Year 2 | Conferences | 3000 | 0 |
| Year 2 | Travel | 15000 | 0 |
| Year 2 | Workshop | 10000 | 0 |
| Total Cost | - | 106000 | 124000 |

**In-kind contributions**:

- XES Setup
- Travel to AXIm

**Financial requests**:

- Setup
- Publications
- Dissemination

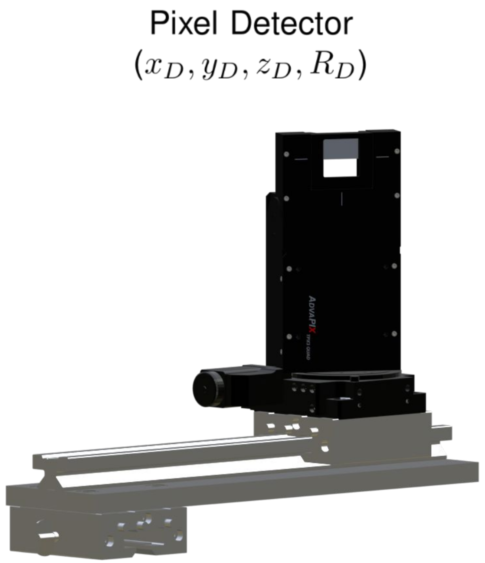
# Support to LNF Services

**Design Services (0.5 Man-Month):**

- **CAD Modeling:** Detailed 3D models for integration support of the **pixel detector** and **motorized stages** with the VOXES setup.

**Mechanical Workshop Services (0.5 Man-Month):**

- **Custom Fabrication:** Precision fabrication and mounting of integration supports to perfectly fit with the existing setup.



# Impact:

- **Advancements in X-ray Beamline Optimization:**
  - Generalized framework for enhanced collaboration and data reproducibility.
  - Open-source software potential.
  - Automation reduces human errors and improves efficiency.
  - Tenfold reduction in acquisition time, leading to cost savings.

- **Social and Technological Benefits:**
  - Improved safety in high-radiation environments.
  - Enhanced efficiency for material science and high-throughput elemental analysis.

# Risks Assessment:

- Inaccuracy of Ray-Tracing Simulations (T1.3)
- Data Integration and Feature Extraction Issues (T1.5)
- Delays in Ordering or Integrating New Equipment (T2.1, T2.2, T2.3)
- Single/Multi-Objective Optimization Complexity (T3.1,T3.2)

# Conclusion

**Challenges in X-ray Beamline Optimization:**

- Complex parameter adjustments requiring **innovative solutions**.

**OPTIMAL Project:**

- Advanced framework using **Bayesian Optimization** and **Reinforcement Learning** with **Machine Learning** for efficient **Multi-Objective optimization**.

**Project Organization and Costs:**

- Structured approach with **detailed planning** and **budget management**.

**Thank you for the attention!**

# SPARE

# Risks Assessment

**1. Inaccuracy of Ray-Tracing Simulations (T1.3)**

• Risk: The ray-tracing simulations may not accurately describe the XES experiment, as they are typically devoted to X-ray beamlines optics and sources, but they are not optimized for simulating mosaic crystals. Such materials have been indeed included in the XOP package only by M. Sanchez del Rio [17].
• Mitigation: Maintain close contact with the developer of the SHADOW-XOP program, Manuel Sanchez del Rio, to seek assistance to improve the accuracy of the simulations.

**2. Data Integration and Feature Extraction Issues (T1.5)**

• Risk: Integrating data from different sources and accurately extracting features from XES spectra using deep learning may present technical challenges.
• Mitigation: Use historical data to bridge gaps between simulated and real-world data.

**3. Delays in Ordering or Integrating New Equipment (T2.1, T2.2, T2.3)**

• Risk: Potential delays in the procurement or integration of the pixel detector and other new equipment could affect project timelines.
• Mitigation: Use a CCD from the VOXES project as a temporary measure to initiate measurements until the pixel detector integration is complete. This CCD, although less efficient and with too small sensitive area, will allow for continued progress on the project.

**4. Single/Multi-Objective Optimization Complexity (T3.1,T3.2)**

• Risk: Balancing multiple objectives (e.g., acquisition time, energy precision, and resolution) in the optimization process may be complex and computationally intensive.
• Mitigation: Regularly evaluate and adjust the optimization strategies based on intermediate results. Engage with experts in optimization and machine learning to refine and enhance the optimization algorithms. Specifically, contact Lucio Anderlini (Florence Section of INFN), whose expertise in artificial intelligence and deep learning can provide valuable insights and support for the project.