International Hybrid Workshop

on

Start-to-End Beamline Optimization for Synchrotron Radiation

and

Free-Electron Laser Facilities

through Artificial Intelligence Approaches

ABSTRACT BOOK



23-24 November 2022

Deutsches Elektronen-Synchrotron (DESY)

Hamburg/Germany

EDITORS

Assoc. Prof. Dr. Bora Ketenoğlu

Assoc. Prof. Dr. Gazi Erkan Bostancı

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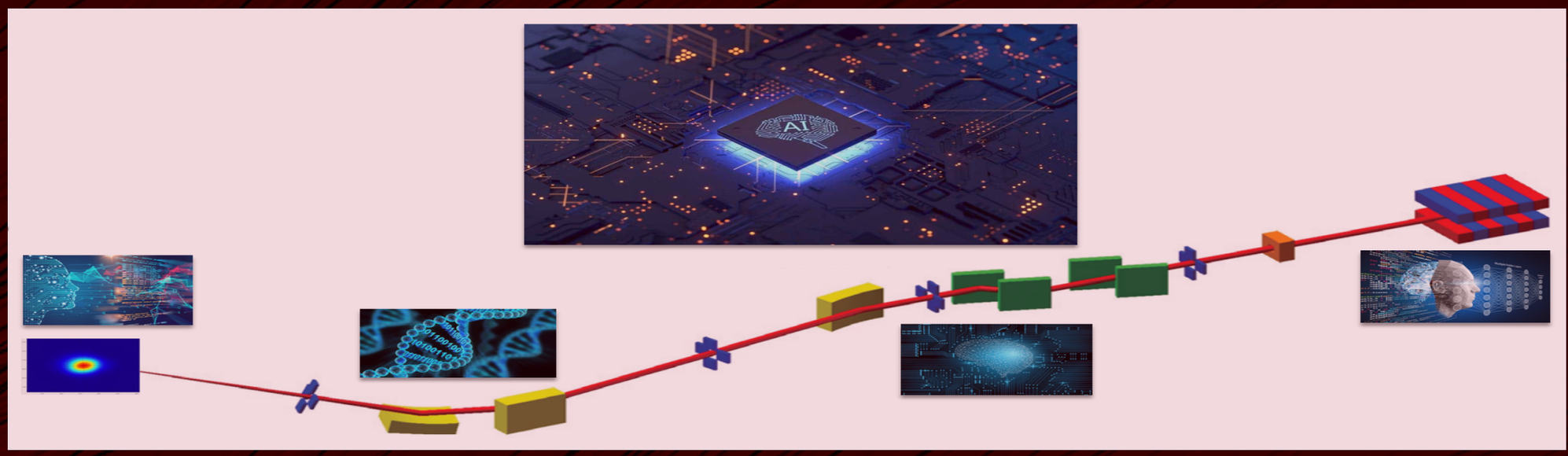

- **The international workshop principally aims to bring "SR & FEL beamline scientists, computer engineers and physicists" together on a dedicated interdisciplinary scientific research basis.**
- **Development and validation efforts on the software GASOLINE (Genetic Algorithms based Synchrotron radiation Optimization for an X-ray beamLINE) will be discussed in detail.**
- **Beamline scientists' comments and recommendations on the international bilateral cooperation project GASOLINE, which is jointly funded by TÜBİTAK (Turkey) and BMBF (Germany), will be adapted to the software for a broad range of SR and FEL beamlines.**

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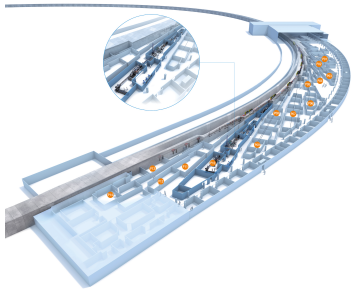

The International GASOLINE Project

Bilateral Cooperation within BMBF (Germany) and TÜBİTAK (Turkey)

Genetic Algorithms

Genetic Algorithms based Synchrotron radiation Optimization for an X-ray beamLINE

Turkish Side (Supporting Foundation#, University and Collaborators)

The Scientific and Technological Research Council of Turkey (TÜBİTAK#)

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Germany Side (Supporting Foundation#, Research Institute, University and Collaborators)

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Foreword

Since accelerator-based 3rd and 4th generation light sources are unique tools in natural sciences research, they provide miscellaneous beamlines for cutting-edge-technology user experiments. In this respect, rapid alignment of beamline components (e.g. mirrors, lenses and monochromators) is a big concern for many scientists. On account of this, the "International Hybrid Workshop on Start-to-End Beamline Optimization for Synchrotron Radiation and Free-Electron Laser Facilities through Artificial Intelligence Approaches" is organized to bring SR & FEL beamline scientists, computer engineers and physicists together on a dedicated interdisciplinary scientific research basis. During the Workshop, development and validation efforts on the software "Genetic Algorithms based Synchrotron radiation Optimization for an X-ray beamLINE (GASOLINE)" will be discussed in detail. Beamline scientists' comments and recommendations on the international bilateral cooperation project GASOLINE, which is jointly funded by TÜBİTAK (Turkey) and BMBF (Germany), will be adapted to the software for a broad range of SR and FEL beamlines. Consequently, the International Hybrid Workshop at Deutsches Elektronen-Synchrotron (DESY), is organized to be held on 23-24 November 2022 in Hamburg-Germany.

We acknowledge all the contributing foundations, research institutes and universities. In addition, special thanks to all members of the International Scientific Committee and the International Organizing Committee as well as to the speakers for their impressive oral presentations.



Assoc. Prof. Dr. Bora Ketenoğlu

On behalf of the International Organizing Committee

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The International Hybrid Workshop on Start-to-End Beamline Optimization for Synchrotron Radiation and Free-Electron Laser Facilities through Artificial Intelligence Approaches is jointly supported by the “Scientific and Technological Research Council of Turkey (TUBITAK)-2525 Bilateral Cooperation Project under Grant No: 121N023” and the “Federal Ministry of Education and Research (BMBF) of Germany”.

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Speakers

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Bora Ketenoğlu
Gazi Erkan Bostancı
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Merna Tanbkji
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Faruk Coban
Koray Açıcı
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Gesa Goetzke
Annika Eichler
Irem Ulku
Useme Şeyh Saleh
Ahmed Alzaidi
Hans-Christian Wille
Danilo Enoque Ferreira de Lima

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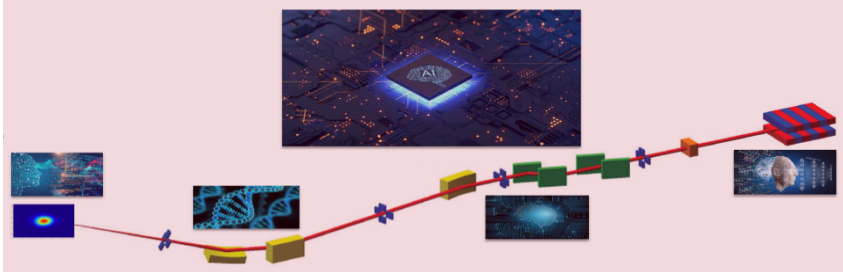

Optimizing KB-Mirror Parameters in XRayTracer with Modified Genetic Algorithm

Ali Can Canbay

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Abstract

Optimizing the experiment setup manually cause prolongation in the time period of the experiment. Furthermore, as a result of increasing experimental studies, the time spend on beamline waiting lists in X-ray facilities will significantly extend. To solve these foreseen problems, it is crucial to optimize the experimental setups before the day of experiment. In this study, KB-mirror parameters were optimized with a modified genetic algorithm using XRayTracer simulation software and the performance results of this new algorithm are given. Considering that the results match with the theoretical expectation and the algorithm is more efficient than the existing ones, it is seen that this technique can also be used in more complex experimental setups.

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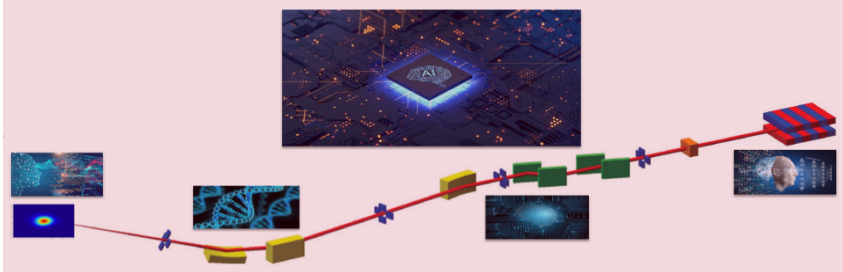

Type IV Secretion System Effector Protein Prediction with Machine Learning Approaches

Koray Açıcı

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Abstract

Extensive research has been done on bacterial secretion systems, as they can pass effector proteins directly into the cytoplasm of host cells. Accurate prediction of type IV protein effectors secreted by Type IV secretion system (T4SS) is important as they are known to play a remarkable role in a variety of human pathogens. Machine learning algorithms are widely used to predict T4SS effector proteins. Some of them are Naïve Bayes (NB), Support Vector Machines (SVM) and Neural Networks (MLP or NN). Before building a model to predict whether a protein is an effector, a protein must be represented as a vector. There are various approaches for vectorizing a protein to feed the machine learning algorithms. If synchrotron radiation is represented by a vector, it can be classified by utilizing machine learning.

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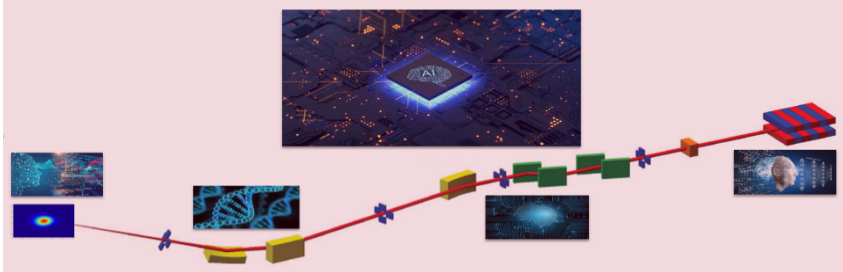

Alignment @ P04

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Abstract

The high brilliance XUV beamline P04[1] of PETRA III combines high flux with high resolving power at a focus size of 10x10 µm^2 for users of the open ports. Hence there is a high demand for an accurate alignment with respect to the position of the optical elements, as well as the photon energy, photon flux, resolution, coherence, and polarization of the photons.

To achieve these goals different tools for alignment are discussed. Examples for different screens e.g., Ce-YAG are shown, and the different footprints and background features are highlighted. A special device ('Focusfinder') is used for measuring the beam caustic around the focal position. The use of the undulator spectrum for finding the undulator axis is explained in theory and by measurement. The use of white light propagation for the alignment of the plane grating monochromator optics is shown. For the calibration of the photon energy filter absorption edges and gas phase absorption spectra are used. Another special tool at P04 is the angular resolved electron Time-of-Flight spectrometer, 'Cookiebox', which can be used to measure the degree of polarization of the photons while the experiment is measuring in parallel. As a final tool the importance of ray tracing and other synchrotron-based software tools is mentioned.

[1] Viefhaus, J., Scholz, F., Deinert, S., Glaser, L., Ilchen, M., Seltmann, J., Walter, P., and Siewert, F. (2013). Nucl. Instr. and Meth. Phys. Res. A 710, 151–154. 10.1016/j.nima.2012.10.110.

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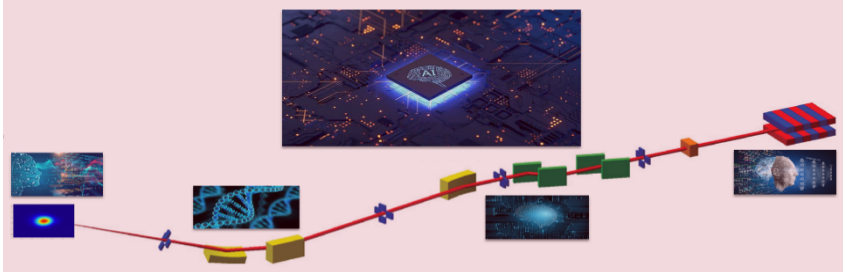

Semantic Segmentation in Remote Sensing Images

İrem Ülkü

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Abstract

Multispectral remote sensing images are one of the important tools that can be used to detect global warming effects. While the use of different spectral information is effective in determining the biophysical and biochemical properties, the images obtained with remote sensing have the ability to cover large areas. Detection of trees in large areas indirectly helps to reduce carbon dioxide emissions resulting from global warming effects. Trees that can reduce carbon dioxide emissions can be identified in large areas and initiatives can be started to increase their numbers where necessary.

Pixel-based detection is possible with semantic segmentation models. At this point, it should be observed how the segmentation performance changes for satellite and aerial multispectral remote sensing images. How segmentation performance will behave in different scenarios depends on the spatial and spectral resolutions. Even a small number of labeled image set works well when spatial resolution is sufficient. The structure of the applied semantic segmentation model, on the other hand, contributes to further increase the performance. In cases where spectral resolution is insufficient, it is not possible to fully utilize the information of multispectral bands and segmentation performance cannot be improved.

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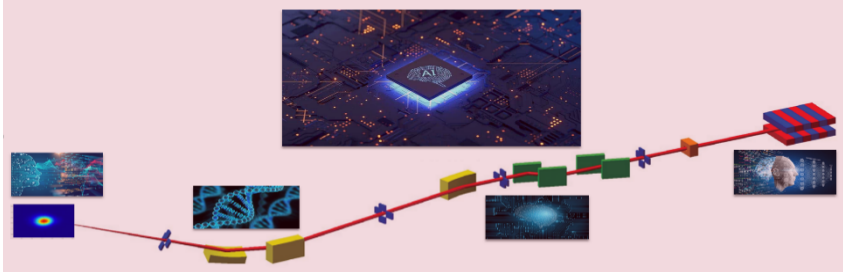

Computation Offloading Problem in Multi-Access Edge Computing

H. Faruk ÇOBAN

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Abstract

In this study, computational transfer methods on mobile edge computing architecture will be examined and method optimization will be made. Cloud computing has made a great impact in the world of informatics in a very short time. Since complex and large operations can be performed outside of supercomputers, it has analysed the characteristics of users with limited resources. Thanks to this solution, some applications such as snapshot processing, sensor data processing, snapshot processing, which were impossible before, have been made possible. However, this new situation also found new problems in itself. Calculation and execution take a certain amount of time to transfer to the cloud and back. Delay, one of the important problems of computer networks, is also hidden here. To solve this problem, mobile edge computing was introduced. Within the scope of the study, rule-based optimization, machine learning and deep learning methods will be applied. When the study is completed, an effective and efficient computational transfer method that can be used in mobile edge computing, which has been tested in both simulation and laboratory environment, will be developed

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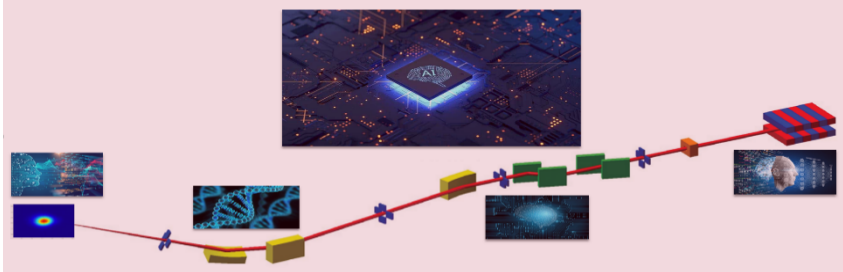

Synchrotron Optimization Using Multi-Objective Evolutionary Algorithms

Gazi Erkan Bostancı

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Abstract

For different reasons, optical elements on a beamline need readjustment for focusing and this process takes days even weeks on some cases which costs valuable beamtime. In this study flux value and spot size of synchrotron radiation are optimized using optical elements. We carried out experiments on X-Ray Tracer Beamline Simulator using Evolutionary Algorithms (EA). These algorithms proved themselves since 70's and have been used for problems with complex mathematical models. EA mimic the nature for their calculations and use the concepts such as reproduction, mutation, recombination, and selection. In essence, EA reward better solutions on random search and use them for the next iteration. Bad solutions are eliminated by selection just like in the nature. EA used in this study are Genetic Algorithm and Non dominated Sorting Genetic Algorithm II as well as two other bioinspired approaches; namely, Particle Swarm Optimization and Artificial Bee Colony. These algorithms were applied on two different experimental setups. One of them optimizes crystal lens position and the other KB mirrors' angles. At first, we used single-objective evolutionary algorithms and checked spot size or flux values separately. Every algorithm configuration is run several times for Monte Carlo simulations since these processes generate random solutions and the simulator also produces solutions that are stochastic. After the comparison multi-objective evolutionary algorithm NSGA II is run for both objectives which are minimum spot size and maximum flux on the lens experiment. The results are shared along with a discussion.

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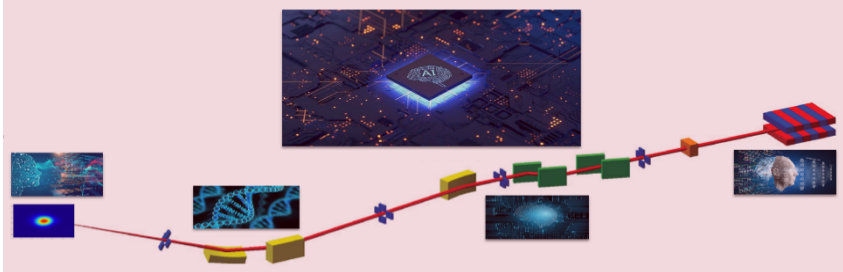

Machine Learning Methods for an Improved Evaluation of FEL Diagnostic Data

Gesa Goetzke

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Abstract

We introduce beta-variation autoencoders to evaluate single-shot diagnostic data from FELS. These artificial neural networks can find key information in a data set without expert knowledge. We demonstrate the application of this type of network to data from the online photoionization spectrometer OPIS and the transverse deflection structure Polarix, both at FLASH at DESY.

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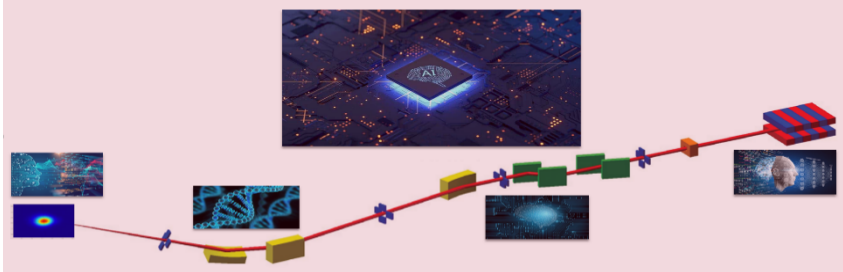

Automatic Serial Femtosecond Crystallography Online Data Analysis with Bayesian Optimization

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Abstract

Photon science experiments in large facilities require fast feedback during data acquisition, so that scientists may adapt he experimental setup if it is not ideal or detect and correct issues early. Several tools are available, but they often require expert input, which is not always available while performing the experiment. In some cases, the availability of such fast online feedback system may be determinant to the success of that scientific endeavour. We propose a system which reduces this barrier in the case of Serial Femtosecond Crystallography, thereby automating the online analysis infrastructure for such experiments.

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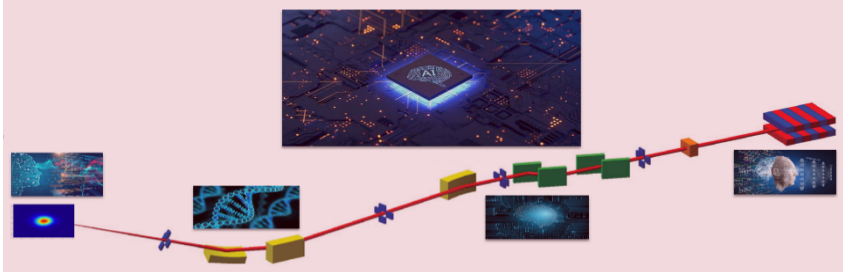

Generative Models for Fast Simulation of the Calorimeters in High Energy Physics

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Abstract

Simulation in High Energy Physics (HEP) places a heavy burden on the available computing resources and is expected to become a major bottleneck for the upcoming high luminosity phase of the LHC and for future Higgs factories, motivating a concerted effort to develop computationally efficient solutions. Methods based on generative machine learning methods hold promise to alleviate the computational strain produced by simulation while providing the physical accuracy required of a surrogate simulator.

In this contribution, an overview of a growing body of work focused on simulating showers in highly granular calorimeters will be reported, which is making significant steps towards realistic fast simulation tools based on deep generative models. Progress on the simulation of both electromagnetic and hadronic showers will be presented, with a focus on the high degree of physical fidelity and computational performance achieved. Additional steps taken to address the challenges faced when broadening the scope of these simulators, such as those posed by multi-parameter conditioning, will also be discussed.

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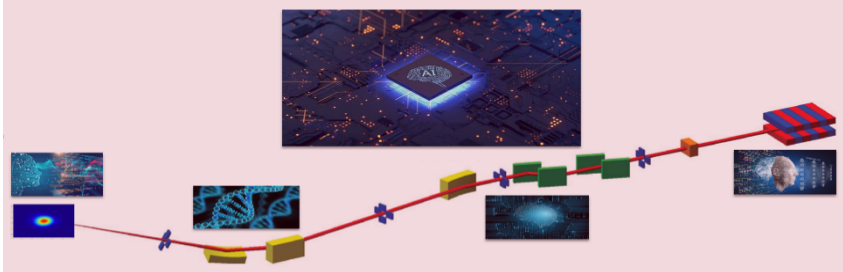

A Comparative Review of X-Ray Beamline Components Employed in SR And FEL Facilities Worldwide

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Abstract

High-brilliance X-ray sources are powerful probes to investigate the properties of matter down to the sub-angstrom scale and on time scales that can extend below a femtosecond. In this article, an introductory overview of the worldwide SR and FEL facilities is mentioned.

The optical components that are used to define the SR ray envelope and tune the beam quality and quantity for experiments are explained briefly. For the X-Ray Optical Elements, we mentioned about: Mirrors, Crystal Monochromators, Grating Monochromators, Focusing Optics and Transport of High Harmonic Radiation. For several experiments, focusing the x-ray beam to a small spot is desirable to increase the photon density at the sample position. This means that the lens apertures should be as large as the beam to collect as many photons as possible. High resolution x-ray mirrors are usually built in KB geometry.

In addition to the optical elements, the photon beam transport includes other elements required for control and diagnostics of the x-ray beam and for vacuum control purposes. Other beam transport elements are mentioned in this article as follows: Safety shutter, slit system, Gas absorber system, Fast shutter for pulse selection and the Beamline vacuum system.

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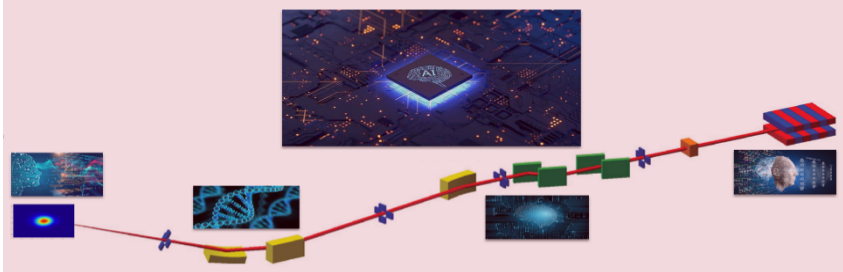

An Application of Artificial Intelligence Approach: Disease Detection via Computer Vision

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Abstract

Artificial intelligence, after its success in other disciplines of sciences, has made the medical approach such as medical imaging and diagnosis swifter. Several success stories are available in the literature where the AI tools are used to improve the results of diagnostic as well as the interventional radiology. Computer-aided diagnosis have stumbled rapidly in the last few years. One of foremost step in computer-aided diagnosis is organ classification and segmentation. Mostly the interpretations of abdominal images are being done by medical experts or radiologists. Image interpretation by human experts is quite limited due to its subjectivity, complexity of the image, extensive variations exist across different interpreters, and fatigue. Deep learning provides exciting solutions with good accuracy for medical imaging and is seen as a key method for future applications in medical field. Urgency of deep Convolutional Neural Networks (CNN) tends to provide better classification in abdominal imaging analysis as compared to traditional models. This approach presents the state of the art of abdominal images for classifying abdominal organs based on deep learning. First, I described background of AI as well as its modalities (Machine Learning and Deep Learning). Then, I reviewed the techniques of deep learning for image segmentation, object detection, classification, and other related tasks for disease detection. In the last section, I have discussed current market challenges and the future recommendations.

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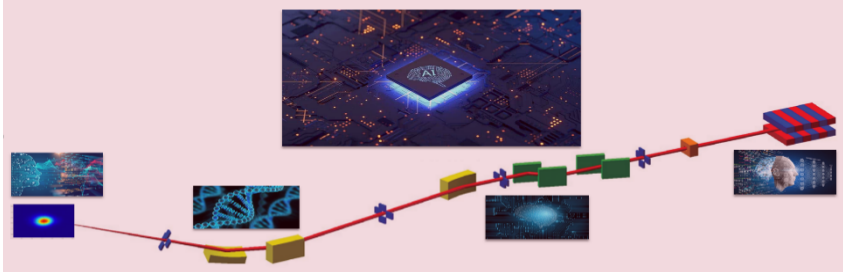

Artificial Intelligence / Machine Learning Applications in X-ray Beamline Optimization for SR and FEL Facilities: A Brief Overview

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Abstract

The term of Artificial Intelligence applies broadly to a collection of computational algorithms and techniques that train systems from raw data rather than a priori models. AI techniques are now technologically mature enough to be applied to particle accelerators, we review in this presentation AI techniques currently being investigated at particle accelerator facilities, and we place specific emphasis on active research efforts and promising exploratory results of optimizing the x-ray beamline for SR and FEL using AI algorithms.

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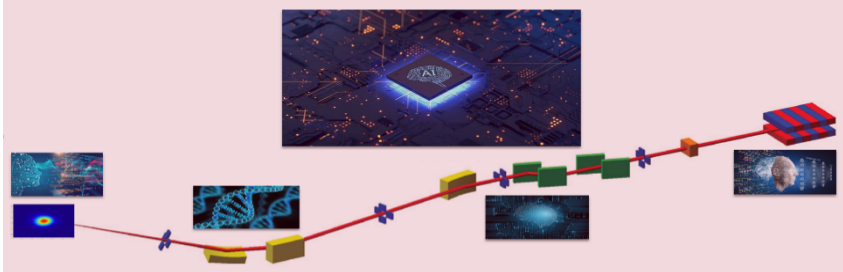

Data Recognition and Beamline Automation

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Abstract

X-ray Absorption Spectroscopy (XAFS) is a versatile method in the application of synchrotron radiation in science, and many different tasks still require human interaction in the collection of data. This can become quite time-consuming, which is a reason to implement better automation in order to accelerate processes and to reduce the risk of human errors.

One possible application is the alignment of samples: In many cases, samples with slightly different compositions are studied. Right now, these samples are aligned manually in the x-ray beam, and the positions of the samples are then copied manually into a script for measurements. The amplification of detectors is also adjusted individually for each sample. These steps can be accelerated by using pictures and intelligent algorithms in order to determine positions of samples on the sample holder, align these samples, determine the amplification, and to determine the quality of the spectra. Especially the last step will profit by a machine-learning process. In other cases, samples are destroyed by the intense x-ray flux, which can break bonds in organic compounds. Therefore, it is necessary to compare spectra which are measured at different times, and to determine if changes in the line-shape are caused by radiation damage or if it is just different noise.

Another application is the study of processes under in-situ conditions or in dependence of several parameters like spatial mapping or inelastic scattering measurements. Sometimes, it is quite time-consuming to search the entire parameter space in order to determine, under which conditions changes in the sample occur or where interesting features can be detected. This can be done in a better way with an algorithm, which looks at different points in parameter space and determines the next point based on previous results. First applications of such algorithms have been implemented by *M.M. Noack et al.*[2]

[2] M.M. Noack et al., Gaussian Processes for Autonomous Data Acquisition at large-scale Synchrotron and Neutron Facilities, Nature Reviews Physics **3** 685-697 (2021) https://doi.org/10.1038/s42254-021-00345-y

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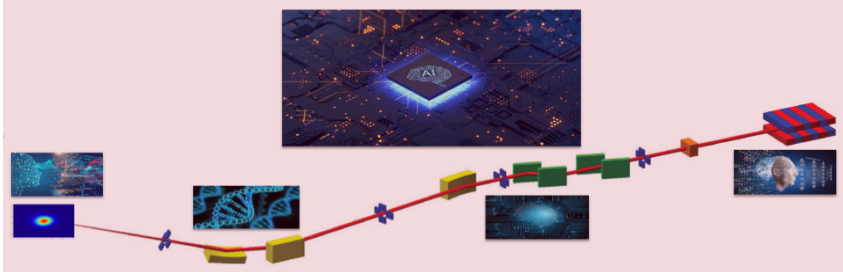

The ROCK-IT Project – An Automated Operando Catalysis Beamline

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Abstract

Together with partners from the Helmholtz-Zentrum Berlin, Helmholtz-Zentrum Dresden-Rossendorf and the Karlsruhe Institute for Technology, DESY successfully applied for Helmholtz funding for a demonstrator beamline with a focus on automation of complex *operando* studies in catalysis research. The 3-year project will start in 2023 and includes automation and remote control of the beamline but also optimisation of the chemical processes of *operando* studies supported by online analysis using machine learning (ML). At DESY, the beamline P65 for X-ray absorption spectroscopy will be upgraded during the project. Besides some new instrumentation the main focus of the project is on developing new control and analysis software and developing the ML code. This project, called ROCK-IT (remote, operando controlled, knowledge-driven, IT-based), addresses these challenges by the intention to provide solutions to improve the efficiency of catalysis research, tailor-made, yet composed of generic building blocks portable enough to be applicable to a wide range of measurements.

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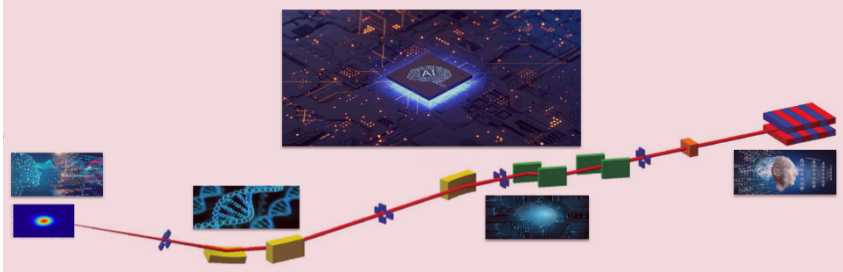

Parameter Optimization of Button Type BPM Using Bio Inspired Optimization Methods

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Abstract

Beam Position Monitors (BPM) are one of the most important diagnostics tools to diagnose entire system and they are used to determine position of beam inside the beam-pipe This study presents bio-inspired methods known as Particle Swarm Optimization and Evolutionary Algorithms in order to design RF antennas for button-type BPMs. Such optimization methods do not require prior knowledge about the solution, rather use a fitness function to choose among candidates that are promising to yield better solutions through a heuristic process. In this study, we focused on optimizing the geometric properties of BPM antennas such as diameter, thickness, and gap. Our results show that the antenna parameters obtained using these multiple objective approaches present suitable SNR and linearity values for signal processing.

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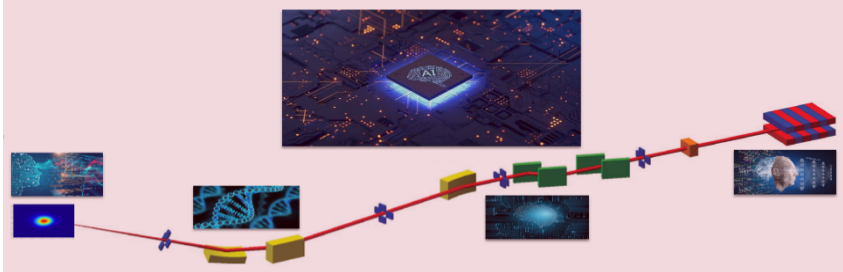

The GASOLINE Project Overview

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Abstract

The international bilateral cooperation project entitled “Genetic Algorithms based Synchrotron radiation Optimization for an X-ray beamline (GASOLINE)” has been jointly funded by Bundesministerium für Bildung und Forschung (BMBF) of Germany and the Scientific and Technological Research Council (TÜBİTAK) of Turkey for two years period. A goal of the project is to develop a “user-friendly software with web application” for beamline scientists. In this respect, the software GASOLINE that is under development phase, principally aims automatic optimization of SR and FEL beamline components through Artificial Intelligence approaches. Development and validation efforts on the software GASOLINE will be discussed in detail. Finally, beamline scientists' comments and recommendations on the project will be adapted to the software for a broad range of SR and FEL beamlines.

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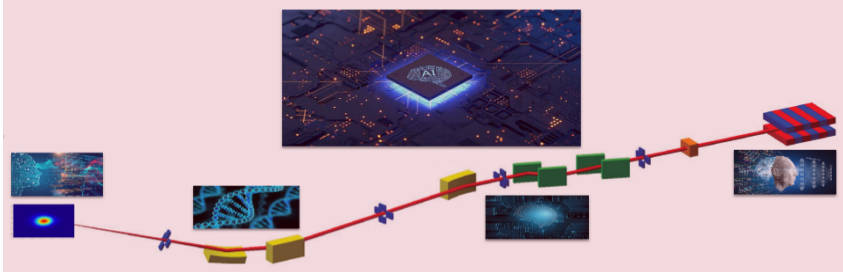

Overview of The ML Activities in the HIR^3X Project

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Abstract

In this talk an overview about machine learning activities in the machine division at DESY are given. The activities are categorized according to the four topics of (i) data acquisition and data analysis, (ii) surrogate modelling, simulation, and digital twins, (iii) fault diagnosis and supervisory control and (iv) optimization and feedback control algorithms. These topics cannot be considered on their own but are strongly interlinked as the first on data acquisition but also the second on modelling are prerequisites for the other.

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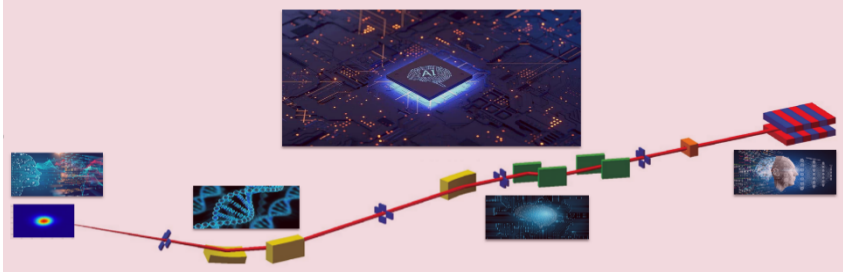

Welcome to DESY

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Abstract

Welcome address and overview of DESY's accelerator-based photon sources as well as current upgrade programs and newly established scientific institutions on the DESY campus.

List of Registrants

1. **Adnan Sahin Karaca**- Ankara University
2. **Ahmed Alzaidi**- Ankara University
3. **Alexander Schökel**- Deutsches Elektronen-Synchrotron (DESY)
4. **Ali Can Canbay**- Ankara University
5. **Andrey Gruzinov-** Deutsches Elektronen-Synchrotron (DESY)
6. **Arif Öztürk**- TOBB University of Economics and Technology
7. **Arman Davtyan** – European XFEL
8. **Ayhan Aydin**- Ankara University
9. **Baran Tan**- Ankara University
10. **Betul Bostancı**- Havelsan Inc.
11. **Beyzanur Aka**- Ankara University
12. **Bora Ketenoğlu**- Ankara University
13. **Burak Dağlı**- TOBB University of Economics and Technology
14. **Can Dokuyucu**- Turkish Accelerator and Radiation Laboratory (TARLA)
15. **Christian Grech**- MXL (XFEL)
16. **Danilo Enoque Ferreira De Lima**- European XFEL
17. **David Meier**- Helmholtz Zentrum Berlin (HZB)
18. **Didem Ketenoğlu**- Ankara University
19. **Döneay Pirişan**- Ankara University
20. **Ece Çizen**- TOBB University of Economics and Technology
21. **Ece İlkay Sungur**- Middle East Technical University (METU)
22. **Ege Uysal**- TOBB University of Economics and Technology
23. **Egor Sobolev**- European XFEL
24. **Emin Yüksel**
25. **Emre Gürsoy**- Technische Universität Hamburg (TUHH)
26. **Engin Eren**- FLC (Ftx Fachgruppe Sft), DESY
27. **Erol İlker İlgün**- Turkish Accelerator and Radiation Laboratory (TARLA)
28. **Faruk Çoban**- Ankara University
29. **Fatma Elali**- Ankara University
30. **Fatma Hanım Subaşı**- Ankara University
31. **Felix Möller**- Helmholtz Zentrum Berlin (HZB)
32. **Gamze Aydo Aydoğan**- Pamukkale University
33. **Gazi Erkan Bostancı**- Ankara University
34. **Georg Spiekermann**- ETH Zürich
35. **Gesa Inken Caroline Goetzke**- Deutsches Elektronen-Synchrotron (DESY)
36. **Ghina Allah Saadedeen**- Ankara University
37. **Göksu Yücel**- Ankara University
38. **Günce Göç**- Ankara University
39. **Halil Kolatan**- Ankara University
40. **Hamdi Vural**- Turkish Accelerator and Radiation Laboratory (TARLA)
41. **Hande Toffoli**- Middle East Technical University (METU)
42. **Hans-Christian Wille**- DESY FS- PETRA -S
43. **Hasan Sansar**- Ankara University & Turkish Accelerator and Radiation Laboratory (TARLA)
44. **Hlynur Gretarsson**- Deutsches Elektronen-Synchrotron (DESY)
45. **İlkay Türk Cakır**- Accelerator Technologies Institute, Ankara University
46. **İlkay Zamur-** Ankara University
47. **İrem Ülkü**- Ankara University
48. **Jan Garrevoet**- Deutsches Elektronen-Synchrotron (DESY)
49. **Jianhui Chen**
50. **Jörn Seltmann**- Deutsches Elektronen-Synchrotron (DESY)
51. **Kaan Baykal**- TOBB University of Economics and Technology
52. **Kai Bagschik**- DESY FS-PETRA PETRA IV
53. **Kemal Shafak**- Cycle GmbH

54. **Ken Vidar Falch**- Deutsches Elektronen-Synchrotron (DESY)
55. **Koray Açıcı**- Ankara University
56. **Kristina Dingel**- University of Kassel
57. **Kutlu Şahbaz**- Ankara University
58. **Luca Gelisio**- European XFEL
59. **Mads Bregenholt Jakobsen** - Deutsches Elektronen-Synchrotron (DESY)
60. **Mahdi Mohammadi Bidhendi** - Deutsches Elektronen-Synchrotron (DESY)
61. **Mahmoud Asfour**
62. **Manuel Harder** - Universität Hamburg / Deutsches Elektronen-Synchrotron (DESY)
63. **Martin Seyrich** - Centre for X-Ray and Nano Science, Deutsches Elektronen-Synchrotron (DESY)
64. **Mehmet Serdar Güzel** - Ankara University
65. **Merna Tanbkji** - Ankara University
66. **Metin Arslan**- Roketsan
67. **Michael Martins**- Universität Hamburg
68. **Michael Meyer**- European XFEL
69. **Nihat Emre Yüzügüldü**- TOBB University of Economics and Technology
70. **Oleh Ivashko**- FS-PETRA-D (FS-PET-D Fachgruppe P072)
71. **Ömer Yavaş**- Ankara University
72. **Osman Emre Delialioğlu**- TOBB University of Economics and Technology
73. **Peter Feuer Forson**- Helmholtz Zentrum Berlin (HZB)
74. **Ragid Ala**- Ankara University
75. **Refik Kuyrukçu**- Turkish Accelerator and Radiation Laboratory (TARLA)
76. **Regina Biller**- Deutsches Elektronen-Synchrotron (DESY)
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80. **Siarhei Dziarzhytski**- Deutsches Elektronen-Synchrotron (DESY)
81. **Useme Şeyhsaleh**- Ankara University
82. **Yue Sun**- European XFEL
83. **Zaid A Hasan Hasan-** University of Michigan
84. **Zhong Yin**- Tohoku University
85. **Özkan Şahin**- Bursa Uludağ University