2nd International Hybrid Workshop (IHW)

on

Start-to-end Beamline Optimization for Synchrotron Radiation and Free-Electron Laser Facilities through Artificial Intelligence Approaches

ABSTRACT BOOK

17-18 January 2024

Deutsches Elektronen-Synchrotron (DESY)
Hamburg/Germany

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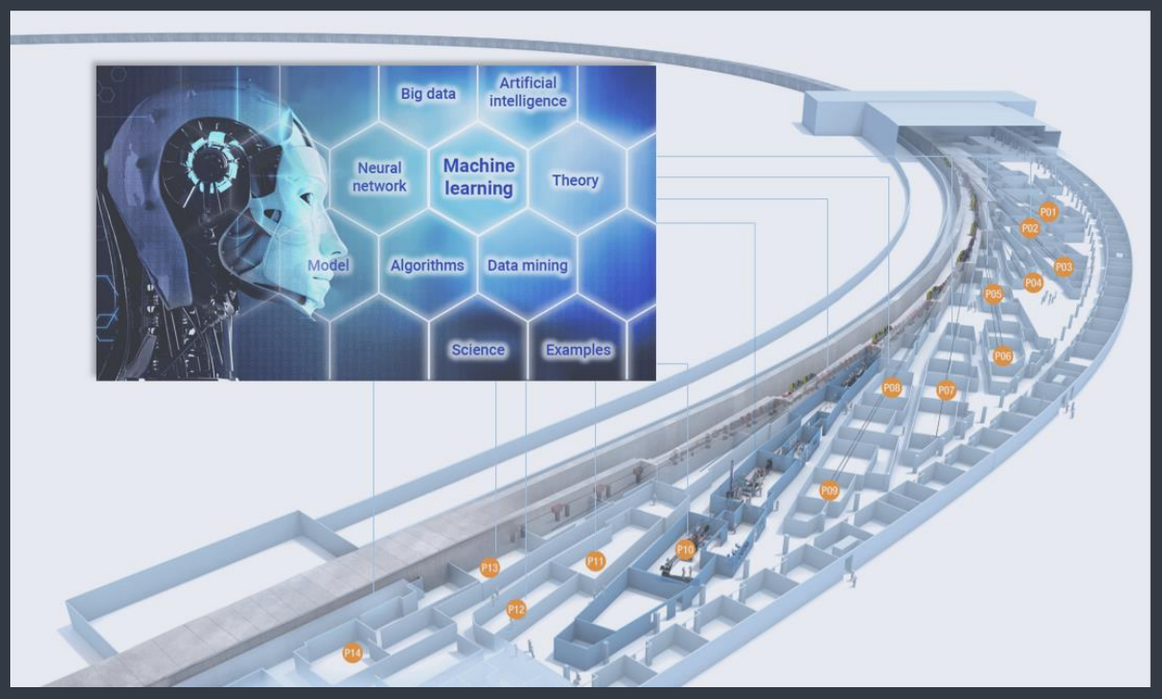

The International Hybrid Workshop (IHW) series aim to bring "photon beamline scientists of SR and FEL facilities, physicists and computer engineers" together on a dedicated interdisciplinary scientific research basis.

Current status and recent progresses on development and validation efforts for the GASOLINE software will be presented in detail.

Comments and recommendations on future prospects for the international bilateral cooperation project between TÜBİTAK of Turkey and BMBF of Germany, entitled "Genetic Algorithms based Synchrotron radiation Optimization for an X-ray beamLINE (GASOLINE)", will be discussed.

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Metin

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Foreword

Accelerator-based light sources with improving radiation characteristics and advancements in the experimental techniques offer a wide application area in natural sciences researches. The design of synchrotron and FEL beamlines is challenging due to the large numbers of degree of freedoms in the chain of optical components, the photon properties at the source and the electron dynamics in the particle accelerator. For example, the slightest change in the position of even one of the components in the beamline can cause large fluctuations in the flux, position or energy resolution of the beam that interacts with the sample. When the mirrors and/or crystals in the beamline are adjusted to cover different energy ranges, related optical components also need to be optimized, otherwise the flux will decrease significantly. In some cases, beam position shifts for some reasons which reduces the flux at the sample position. In the case of all these and similar situations, the beamline needs to be re-optimized. Usually, all optical elements throughout the synchrotron beamlines are aligned individually which takes more time. This is where the need for optimization methods finds its justification. The work presented in our project is a contribution to an approach to beamline design than can accommodate an arbitrary number of optimization requirements.

Within the framework of the international bilateral cooperation project "Genetic Algorithms based Synchrotron radiation Optimization for an X-ray beamLINE (GASOLINE)", which is jointly funded by TÜBİTAK (Turkey) and BMBF (Germany), it is aimed to pave the way for scientific collaboration between the scientists and researchers of the both parties working in the area of accelerator-based light sources and computational intelligence. Within the scope of the project, "International Hybrid Workshop on Start-to-End Beamline Optimization for Synchrotron Radiation and Free-Electron Laser Facilities through Artificial Intelligence Approaches" is organized for the second time to bring SR & FEL beamline scientists, computer engineers and physicists together on a dedicated interdisciplinary scientific research basis. Consequently, the International Hybrid Workshop is organized to be held on 17-18 January 2024 in at Deutsches Elektronen-Synchrotron (DESY), Hamburg-Germany.

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

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Faiza Iftikhar

Zhong Yin

Saima Abdullah

Fatima Zehra Ünal

Koray Açıcı

Adnan Şahin Karaca

Nadia Kanwal

Workshop Program

17 January 2024

10:00	**The GASOLINE Project Overview** *Didem Ketenoğlu* 10:00 - 10:30
	Concluding Remarks on the GASOLINE Project *Gazi Erkan Bostancı* 10:30 - 11:00
11:00	**AI-driven Medical Imaging: Excerpts from the research project KI@CAU-Datencampus** *Stephan Schneider* 11:00 - 11:30
	In-vacuum X-ray Undulator based Synchrotron Radiation Optimization within the scope of GASOLINE Project *Bora Ketenoglu* 11:30 – 12:00
12:00	**Lunch** 12:00 - 13:30
13:00	
	Artificial Intelligence and X-Ray Absorption Spectroscopy *Wolfgang Caliebe* 13:30 - 14:00
14:00	**Denoising attempts with SAXS data via Deep Learning** *Engin Eren* 14:00 - 14:30
	Integrating Artificial Intelligence Methods for Precision Agriculture Applications Based on Remote Sensing Images *İrem Ülkü*
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	Decoding the Patterns of Human Behavior: A Locally Weighted Machine Learning Approach for Complex Human Activity Recognition *Tunc Asuroglu*
	Deep learning techniques to enhance the performance of optical sensors *Faiza Iftikhar* 15:45 - 16:15
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Following ultrafast dynamics with soft X-ray spectroscopy *Zhong Yin*

10:00 - 10:30

An IoT based Data Aggregation Mechanism for Cotton WhiteFly Pests *Saima Abdullah*

10:30 - 11:00

11:00

Deep Learning based Approach for Multilabel Genre Prediction *Fatima Zehra UNAL*

11:00 - 11:30

Coffee Break

11:30 - 11:45

Enhancing Femoral Neck Fracture Detection in X-ray images with a Genetic Algorithm-Optimized Deep Learning Model
Koray Açıcı

12:00

Lunch

13:00

12:15 - 13:30

Evolutionary Approaches For Beamline Optimization – Analyzer Study *Adnan Sahin Karaca*

13:30 - 14:00

14:00

Securing Visual Data Processing: Harnessing Deep Learning for Privacy and Security *Nadia Kanwal*

14:00 - 14:30

Oral Presentation Abstracts

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- Concluding Remarks on the GASOLINE Project
  Gazi Erkan Bostancı
- AI-driven Medical Imaging: Excerps from the research project KI@CAU-Datencampus
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The GASOLINE Project Overview

Content

The idea of our project is constructed on the optimization of synchrotron radiation based hard and soft X-ray beamlines through multiple objective Genetic Algorithms. In addition to Multiple Objective Evolutionary Algorithms and variants, two other bio-inspired optimization methods including Particle Swarm Optimization (PSO) and Artificial Bee Colony Optimization (ABC) are used to optimize the main beamline components including the source (undulator/wiggler) to obtain the required synchrotron radiation characteristics such as beamsize, beam position, flux and energy resolution for dedicated user experiments. In this context, as a first step the input parameters of the main optics and source device constituting a synchrotron beamline operating at hard and soft X-ray region are defined for the Genetic Algorithms optimization and in this way, the optimum radiation characteristics are obtained by varying the input parameters in a reasonable range.

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Presenter: KETENOGLU, Didem (Ankara University)

In-vacuum X-ray Undulator based Synchrotron Radiation Optimization within the scope of GASOLINE Project

Content

Since accelerator based light sources are cutting-edge-technology tools in natural sciences research of the 21st Century, they provide unique user experiments by superior radiation characteristics. On account of this, rapid & high-precision alignment of photon beamline components (including design and optimization of the undulator as a matter of course), is a big concern for many beamline scientists. In this respect, a hybrid in-vacuum X-ray undulator driven by a 6 GeV synchrotron, is optimized through Evolutionary Algorithms (EAs). It is shown that the EA results provide promis- ing design & optimization estimations for photon beamline scientists.

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Presenter: KETENOGLU, Bora (Ankara University)

Denoising atempts with SAXS data via Deep Learning

Content

Research on the application of small-angle x-ray scattering (SAXS) method, using x-ray free-electron laser (XFEL) images, utilizes normalizing flows for the inversion of experimental X-ray scattering images. One of the main challenges lies in the inversion of such experimental scattering images, which contain various artifacts such as parasitic scattering, slit scattering, beamstop, and detec- tor background. These artifacts pose a significant domain shift for the neural network used in the inversion process. Parasitic scattering typically appears as a Gaussian-shaped cluster around the primary beam, accompanied by scattered photons in the vicinity. Slit scattering manifests as streaks around the primary beam, while the beamstop obstructs the main beam entirely, resulting in a lack of signal. The detector background refers to an offset with some underlying structure. Currently, the simulated dataset is being modified to incorporate these artifacts. However, this approach may not be sustainable in the future, as the exact characteristics of the artifacts are un- known in advance, and there is limited time to model them during the experiment. Hence, the intention is to collaborate in developing a resilient feature extractor capable of extracting features from both simulated and experimental data, even in the presence of unknown artifacts. These extracted features will subsequently be utilized for the inference process in the primary neural network responsible for inversion.

We aim to address the problem by using contemporary deep learning techniques. At present, we are exploring two potential approaches: one involves learning representation through β-VAE, while the other entails utilizing image-to-image translation methods such as CycleGAN and pix2pix.

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Presenter: EREN, Engin (IT (Research and Innovation in Scientific Co))

Evolutionary Approaches For Beamline Optimization – Analyzer Study

Content

The alignment of each analyzer position in X-ray Raman Scattering (XRS) setup requires a great deal of time, therefore using the optimization approaches is necessary. In this study, Non-dominating Sorting Genetic Algorithm-II (NSGA-II) was used on 101 images from detectors while positioning each analyzer. The images first filtered through 2D Gaussian filter to obtain a cloud of dots repre- senting the spread of the X-ray, then spot size and flux values were optimized first separately and later simultaneously. Flux is related to the amplitude of the Gaussian distribution of the spread of the rays, whereas spot size is related to the sigma values on the vertical axis x and the horizontal axis y. The first results show that minimum sigma-x, sigma-y values and maximum amplitude are provided at different positions, thus NSGA-II is run on multi-objective mode. Pareto set is found with six elements.

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Presenter: KARACA, Adnan Sahin (Ankara University)

Integrating Artificial Intelligence Methods for Precision Agriculture Applications Based on Remote Sensing Images

Content

Analyzing a significant amount of remote sensing data obtained through Unmanned Aerial Vehi- cles (UAVs) and satellite-based technologies for Precision Agriculture (PA) applications involves artificial intelligence (AI) methods. AI applications aim to enhance crop yield efficiently while min- imizing input costs and environmental impacts in optimal locations. Designing the most suitable deep learning architecture, considering the requirements of PA, is crucial. This architecture should maximize the utilization of multispectral band images found in remote sensing data, offering signif- icant information. However, specific AI techniques, particularly Convolutional Neural Networks (CNNs), experience delays in inference. There is limited research on AI algorithms that integrate into UAVs for real-time PA applications. Therefore, the designed CNN architecture should aim to reduce inference time and establish a balance between speed, memory, and accuracy. This study evaluates the performance of various CNN architectures, considering all PA application require- ments for detecting objects such as trees, crops, and wheat yellow-rust disease. The final discussion covers modifications relevant to achieving an optimal CNN architectural design for PA.

Primary author: Dr ULKU, Irem

Presenter: Dr ULKU, Irem

Enhancing Femoral Neck Fracture Detection in X-ray images with a Genetic Algorithm-Optimized Deep Learning Model

Content

Femoral fractures, a growing threat to the elderly, are predicted to double by 2050. Early diag- nosis and intervention are crucial for joint protection, quality of life, and mobility after surgery. However, misdiagnosis triggers a cascade of delayed treatment, prolonged recovery, and spiralling costs, impacting both patients and healthcare systems.

Deep learning is revolutionizing medical image processing, transforming diagnosis and treatment by extracting hidden patterns from medical scans. Its precision in fracture detection minimizes misdiagnosis, reducing unnecessary procedures and hospital stays, leading to significant cost sav- ings for patients and healthcare systems.

The success of a deep learning architecture is tightly dependent on the values of its hyperparameters. It is possible to increase the performance of a current model by selecting hyperparameters with a genetic algorithm. In our study, we achieved a 1.6% performance boost, in terms of accuracy, for an existing CNN model using a genetic algorithm.

Primary author: AÇICI, Koray (Ankara University)

Presenter: AÇICI, Koray (Ankara University)

Concluding Remarks on the GASOLINE Project

Content

For synchrotron based user experiments, radiation characteristics such as energy resolution, flux and beamsize are of great importance in terms of the feasibility of the experiment. The main diffi- culty stems from adjusting the optics and other components throughout the synchrotron beamline to obtain the required energy resolution, flux and beam position values. The optimum param- eters are determined by manually (remotely) controlling the each element constituting a beam- line, which takes several days even weeks. The main goal of the Genetic Algorithms-based Syn- chrotron radiation Optimization for an X-ray beamLINE (GASOLINE) project was to optimize the synchrotron beamline components operating in the hard and soft X-ray region through Genetic Al- gorithms (GA) in order to achieve the required synchrotron beam characteristics for dedicated user experiments. Two other optimization algorithms were employed in addition to Multiple Objective Evolutionary Algorithms and variants (e.g. GA, NSGAII/III etc.), namely Particle Swarm Optimiza- tion (PSO) and Artificial Bee Colony Optimization (ABC). Results for the optimization processes designed and implemented in the project show that the bio-inspired approaches employed in the project have achieved significant success in the order of seconds execution time.

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Presenter: BOSTANCI, Gazi Erkan (Ankara University)

Decoding the Paterns of Human Behavior: A Locally Weighted Machine Learning Approach for Complex Human Activity Recognition

Content

As life expectancy rises, the elderly care sector faces a looming workforce shortage. Ambient Assisted Living (AAL) systems emerge as a promising solution, with Human Activity Recognition (HAR) as a key component. HAR's ability to automatically track activities empowers comprehen- sive health and well-being assessments, easing the burden on healthcare professionals. Lifelogging and home diary applications further enhance this value by providing valuable insights into daily routines.

Complex activities, however, pose a unique challenge due to their intricate semantic nature. To address this, a machine learning framework that utilizes a single accelerometer sensor to accurately predict complex human activities is proposed. The Locally Weighted Random Forest (LWRF) algorithm, with its hybrid structure and local weighting approach, proves remarkably effective, achiev- ing 91% accuracy for HAR and 91.3% for gender recognition.

This work paves the way for embedding the proposed framework into lifelogging and home diary applications, enabling real-time monitoring of mental status and overall well-being among the elderly. As AAL systems continue to advance, their potential to transform elderly care is undeniable.

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Presenter: ASUROGLU, Tunc (VTT Technical Research Centre of Finland, Finland)

Deep Learning based Approach for Multilabel Genre Prediction

Content

Multilabel classification is a type of classification task in which an instance can be assigned many labels at the same time. Multilabed data can be correctly classified using machine learning and deep learning models. Transfer learning is a machine learning method in which a model trained for specific task is used for different but similar task. In this study, we utilized the transfer learning to overcome the multilabel classification problem. As a case study movie poster image classification is selected because in general, movies have multiple labels/genres. For this purpose, movie images from The Internet Movie Database (IMDB) have been downloaded and used. The popular modern pretrained models have been employed for transfer learning. The iterative stratification technique has been utilized to partition the dataset. Each model has been trained and fine-tuned using this dataset. The performance of each model has been compared taking into account metrics such as AUC, f1-score, precision, loss, and hamming loss.

Primary authors: Mr GUZEL, Mehmet Serdar; UNAL, Fatima Zehra

Presenter: UNAL, Fatima Zehra

Artificial Intelligence and X-Ray Absorption Spectroscopy

Content

X-ray absorption spectroscopy is an established technique in the application of synchrotron ra- diation with applications in many scientific fields. Some scientists are not really familiar with the applications of X-rays in science, others have rather complicated sample environments, which require their full attention. Everybody will profit from an automation of the instrument with control-mechanisms for best beam quality for the experiment, automated sample alignment and control, and preliminary data analysis. These automation procedures can benefit from AI-based algorithms. I will also briefly present an example of data analysis, which is based on an artificial neural net- work.

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Following ultrafast dynamics with soP X-ray spectroscopy

Content

Soft X-ray spectroscopy is a valuable tool for extracting information about the electronic proper- ties of atoms and molecules within a given sample. This technique provides insights into various aspects, including electronic configuration, bonding traits, and the surrounding chemical environment. Nevertheless, a significant portion of pertinent chemical processes, particularly those of a bio-chemical nature, transpire within liquid environments. This circumstance introduces an inherent challenge for experimental endeavors. Consequently, the exploration of molecular systems within their native liquid state necessitates the utilization of advanced experimental setups and sample delivery mechanisms. In this presentation, I will delve into the most recent findings derived from compact photon sources that can be operated on a tabletop. These sources harness powerful femtosecond lasers to drive soft X-ray (SXR) generation, facilitating the practice of time-resolved X-ray absorption spectroscopy (TRXAS). Through this approach, it becomes feasible to monitor dynamic structural and electronic changes in real time.

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Deep learning techniques to enhance the performance of optical sensors

Content

Deep learning (DL) has become widely used in many optical sensor scenarios during the last few years. Notable progress has been made in integrating deep learning algorithms, which improve accuracy and reduce noise in optical sensor data. Optical sensors are a highly promising technol- ogy for modern intelligent sensing platforms. They are used in many different fields, including defence, security, process monitoring, quality prediction, pollution control, and many others. Al- though optical sensors have many applications, they also face many difficulties. These difficulties include the need to create large datasets and the resulting slow processing speeds. On top of this, these sensor technologies are very expensive. To overcome these obstacles, deep learning systems and optical sensor technologies must be strategically integrated. This work presents a systematic review of recent works that have effectively used DL algorithms in optical sensor applications. It not only sheds light on the state of these integrations today but also highlights some encouraging avenues for DL algorithms′continued development in the context of optical sensor applications. Investigating these integrated systems shows how they can be used to get around the problems of processing speed constraints and big datasets, which will ultimately lead to more effective and af- fordable optical sensor solutions. This work also acts as a lighthouse for future research projects, pointing the way towards fresh directions and offering opportunities for creativity in the ongo- ing advancement of DL applications in the field of optical sensors. Overall, this work lays the groundwork for future research and development of AI-enabled optical sensor technologies.

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An IoT based Data Aggregation Mechanism for Coton WhiteFly Pests

Content

Cotton whitefly is an important pest that damages crops and reduces crop yield. An IoT-based data Aggregation methodology is proposed to address the challenges of cotton whitefly pest monitoring and control. Uses sensors and IoT devices provide real-time monitoring and complete control of whitefly pests, while also providing timely information to farmers and supporting decision-making by agronomists. A method of data aggregation has been used to determine the number of pests of cotton whiteflies and the damage caused by them. The data aggregation system is designed to support real-time pest monitoring and control, which is critical for effective pest management and crop protection. This study has demonstrated that IoT-based data collection method has proved useful in detecting and controlling cotton whitefly pests and providing timely information to farm- ers

Primary author: ABDULLAH, Saima (The Islamia University of Bahawalpur) **Presenter:**

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Securing Visual Data Processing: Harnessing Deep Learning for Privacy and Security

Content

In recent times, visual surveillance systems have undergone rapid advancements, exhibiting increased capabilities and widespread integration of artificial intelligence. Concurrently, these surveillance systems have raised concerns by exposing the public to emerging privacy and security risks. Instances of overt misuse of surveillance technologies have surged, prompting the implementation of data privacy regulations such as GDPR in Europe to establish guidelines for responsible data collection and processing.

Despite these regulatory measures, there remains a pressing need for a secure and private approach to train sophisticated machine learning and deep learning algorithms. In this paper, we propose a method that prioritizes privacy in visual surveillance. Initially, we curate a dataset consisting of videos with preserved privacy. The content within these videos is obfuscated using a combination of Gaussian Mixture Model (GMM) and selective encryption techniques. Subsequently, we employ this privacy-preserved dataset to train high-performance object detection models.

Primary author: Dr KANWAL, Nadia (Keele University, UK)

Presenter: Dr KANWAL, Nadia (Keele University, UK)

AI-driven Medical Imaging: Excerpts from the research project KI@CAU-Datencampus

Content

Data-driven decisions open up new fields of action. Such decisions require both subject-specific and information technology expertise. Generally, subject domains have subject-oriented knowl- edge, but not in-depth information technology expertise. The same applies in reverse for IT-related disciplines. The state-funded project KI@CAU-Datencampus brings both disciplines together in the form of tandems and demonstrates the combined development of AI-based solutions in terms of subject and information technology accordingly. This presentation shows two selected examples from neurology and dentistry.

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