GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

**Annual Meeting of the**
**de.NBI Industrial Forum**
Thursday, 19 November 2024

# 5th Annual Meeting of the de.NBI Industrial Forum

# AI Ventures in the Life Science – Challenges, Needs, Opportunities

GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

# Book of Abstracts – Scientific Presentations

19th November 2024, 01:00-04:30 pm (CET)

Virtual Meeting using Zoom

Log-In data will be shared after the registration

# Key Note

## Unseen Challenges: Uncovering the Realities of medical imaging AI

Lena Maier-Hein
Faculty of Medicine, Heidelberg University
Head of Division “Intelligent Medical Systems“, Deutsches Krebsforschungszenturm (DKFZ)
Managing Director „Data Science and Digital Oncology”, DKFZ
Managing Director National Center for Tumor Diseases (NCT), Heidelberg Heidelberg

Abstract:

Advanced medical systems that can capture and interpret sensor data to provide context-sensitive support are reshaping healthcare. Yet, a range of underlying issues—often less visible—pose significant obstacles to the effective incorporation of modern machine learning advancements into clinical settings. Drawing from the work of my research team and extensive international collaborations, I will explore the common challenges within current medical imaging practices and suggest possible solutions. This presentation will emphasize the critical need to rigorously examine each component of the medical imaging workflow—from image acquisition methods to validation processes—to ensure that intelligent imaging systems are ready for true clinical deployment.

# Session A

## Molecular Machine Learning – Transforming Structural Biomolecular Data

Holger Gohlke
Heinrich Heine University Düsseldorf
Forschungszentrum Jülich – Institute of Bio-and Geosciences (IBG)
Bioinformatics / IBG-4

Abstract:

Molecular machine learning is a transformative approach that leverages advanced computational algorithms to decode the complex language of biomolecules, with proteins being a primary focus. By integrating sequence, structural, and functional data, machine learning models can predict protein properties, functions, and interactions with unprecedented accuracy and scalability. Recent advancements in protein-specific foundation models and multimodal architectures have enabled the alignment of diverse data types, such as sequence alignments, 3D structures, and text information, into unified latent spaces. In my talk, I will present our methodological developments for protein structure (TopSuite) and function (TopEnzyme, TopEC) prediction as well as towards a multi-model protein foundation model (OneProt). Putative applications range from enzyme engineering to drug discovery to function annotation. While molecular machine learning provides a powerful and versatile framework for accelerating discoveries in these fields, I will also discuss the challenges of assessing the quality of quickly appearing methods.

# Single-cell and spatial biology in the Era of Genomics and AI

Naveed Ishaque
Head of Computational Oncology, Center of Digital Health, Berlin Institute of Health@Charité
Berlin

Abstract:

Recent advancements in single-cell and spatial transcriptomics have transformed our capacity to dissect molecular and cellular heterogeneity in biomedical research. These technologies are now at the forefront of understanding complex biological systems. In this talk, I will explore how AI-driven methodologies provide unprecedented opportunities to decipher single-cell transcriptional dynamics, offering new ways to model early molecular events that influence development and disease progression. Through these models, we aspire to pinpoint therapeutic interventions that can modify disease-prone cellular trajectories before they manifest as pathology. Spatial transcriptomics further illuminates the molecular and cellular architecture within tissues, capturing both gene expression and spatial cellular organization. This dual insight reveals the intricate communication between cells, tissues, and organs—a foundation for understanding the mechanisms behind health and disease. Yet, while enthusiasm for these technologies is high, integrating AI into their analysis faces considerable challenges, particularly around data management, standardization, and computational scalability. These challenges underscore the need for innovative AI solutions to enable actionable insights from this data revolution. My talk will highlight solutions to some of these obstacles and the transformative potential of AI in advancing precision medicine.

# Session B

## Artificial intelligence to Enable Food and Crop Sustainability

Sebastian Schultheiss
Managing Director
Computomics GmbH
Tübingen

Abstract:

In a world facing unprecedented challenges to food security, AI has emerged as a powerful tool for advancing crop sustainability. Computomics harnesses AI and bioinformatics to transform agriculture by offering data-driven solutions that help breeders and growers adapt to changing climates, optimize crop yields, and reduce environmental impact. Our proprietary models integrate genomic, phenotypic, and environmental data to provide actionable insights, from breeding and crossing recommendations to ideal variety placement taking into account future climate and soil conditions.

By leveraging AI in precision breeding, we identify resilient crop traits that can withstand drought, disease, and other stress factors, making food production more predictable and sustainable. Computomics' tools are designed to serve both traditional and indoor farming, where sensor-driven feedback loops automate lighting, irrigation, and temperature control. Our technology supports breeders in producing varieties tailored for specific climates, reduce input costs, and minimize crop loss. As we continue to expand our AI-driven solutions, Computomics remains committed to empowering agriculture with the tools needed for a resilient and sustainable future in food production.

# Data are health, and digital twins are the future of AI in modern treatments

Christian Stephan
Managing Director
Kairos GmbH
Bochum

Abstract:

Data are crucial for the improvement of healthcare and the implementation of artificial intelligence (AI) in the medical field. With the increasing availability of health data, the potential for improving patient outcomes and healthcare delivery is immense. Digital twins, which are virtual representations of individual patients, have emerged as a promising tool for personalized medicine and predictive analytics. By integrating patient data with digital twin technology, healthcare providers can gain valuable insights as decision support into disease progression, treatment response, and overall patient health. This presentation explores the significance of data in healthcare and the potential of digital twins as the future of AI in medicine. It discusses the opportunities and challenges associated with leveraging health data for AI applications and therefore for support in treatment and diagnostics, as well as the implications for the software as a medical device. The integration of data and digital twins has the potential to revolutionize the way healthcare is delivered, leading to more personalized and effective treatments for patients. However, there are also technical, ethical, regulatory and privacy considerations that need to be addressed to ensure the responsible use of health data. Overall, the intersection of data, health, and digital twins presents exciting opportunities for advancing AI in healthcare and improving patient outcomes.

# arivis Cloud - AI-powered Image Analysis for everyone

Bernhard Fichtl
Product Line Manager
Carl Zeiss Microscopy GmbH
München

Abstract:

arivis Cloud is a web platform that enables researchers & industry customers to leverage the power of Deep Learning without any prior ML/coding experience. It enables collaboration to jointly refine and expand shared models and training datasets, for increased model robustness, and reproducible results. Trained ML models can be easily deployed within the ZEISS SW ecosystem to fully automate the customer workflow. The platform supports the most common microscopy image formats and can be used to solve a wide range of applications independent from any specific field (e.g. life-, materials- and geological-sciences).

# DeepRod: A human-in-the-loop system for automatic rodent behavior analysis

Hanna Behnke
Team Lead AI Project Management
Merantix Momentum GmbH
Berlin

Abstract

AI systems often struggle with data limitations, data distribution shift over time, and a poor user experience. Human-in-the-loop design offers a solution by placing users at the center of AI systems and leveraging human feedback for continuous improvement.

Applying this concept in practice, Merantix Momentum collaborated with Boehringer Ingelheim to develop a tool for automatic rodent behavior analysis at a large scale to enhance pre-clinical safety studies in drug discovery. Addressing the time-consuming and labor-intensive nature of manual behavior categorization, this UX-optimized system integrates AI for complex behavior prediction and active learning to identify rare events. Using the tool, new safety studies can be analyzed for more than 20 behavior types in a day whereas previously the automated detection of these novel behaviors was not possible at all. Furthermore, the system's design allows the scientists to increase the amount of detected behavior types and improve the machine learning model without support from machine learning engineers.

In this talk, we will dive into the human-in-the-loop approach, discussing the underlying machine learning components, the development process, as well as the project's real-world impact. For further insights, you can find our joint publication here: https://doi.org/10.1101/2024.01.04.572506

# Artificial Intelligence and machine learning models for gene regulation databases and services

Philip Stegmaier
Manager Software and Technology Department
geneXplain GmbH
Wolfenbüttel

Abstract

GeneXplain is a provider of leading databases and software with a focus on gene regulation and biomedicine. Artificial intelligence and machine learning models play a role at various places in products and the production process.

Their application encompasses web interfaces enabling users to train models on research data and apply them for predictions, libraries of gene regulatory models accessible through analysis methods and workflows, model recommendation and other areas.

This presentation will showcase several examples of how AI and ML are utilized both within the backend and frontend of geneXplain's products.