KCCM 2025

Proceedings
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Krakow Conference on Computational Medicine

Enhancing Virtual Human Twin with AI solutions

October 15–17, 2025

Editors: Marian Bubak, Ewelina Szymańska-Skolimowska

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FOREWORD

The healthcare system should support personalised disease prevention, diagnosis, and effective treatment for patients. One path to achieving this goal is computational medicine, which utilises high-quality mathematical models of human physiology. These models, in turn, are used as computer simulations to analyse a patient's health situation based on medical data.

Peter Hunter initiated systematic research in this area with the Physiome project, which became the foundation for a series of scientific explorations of the concept of virtual physiological human (VPH). The goal of these efforts is to create a virtual human twin (VHT) – an integrated, multi-scale, dynamic, and interdisciplinary representation of the body's physiology and pathology. A digital twin can support disease risk prediction, recommend dietary and lifestyle changes, treatment planning and monitoring (including surgical procedures), enable the testing of new drugs, and identify therapeutic strategies to improve quality and length of life. In addition to dedicated EU programs, research in this field is coordinated by the VPH Institute.

To put this idea in practice, according to the EDITH VHT Roadmap, we require an inclusive ecosystem of digital twins in healthcare, implementation of a federated cloud-based repository, gathering human digital twin resources such as models, data sets, algorithms, practices, and designing the architecture of a simulation platform to facilitate the transition towards personalised medicine. In this context, AI and data-focused methods, machine learning are perceived not as competitive, but as supportive of existing modelling and simulation techniques.

In Krakow, the Sano Centre for Computational Medicine, Faculty of Computer Science AGH, and Academic Computer Center Cyfronet AGH collaborate in research carried out in computational medicine in above mentioned directions, aimed at providing support to patients and doctors.

Sano, which currently employs 84 people, was established in late 2019 as an international research foundation following the EU Teaming for Excellence competition and the Foundation for Polish Science's International Research Agendas programme; now it is funded through the Polish Ministry of Science and Higher Education. However, the journey began in 2002 with participation in the EU CrossGrid project, followed by 12 further ones at the ACC Cyfronet AGH with the support of the Faculty of Computer Science AGH. Sano's goal is not only excellent science, as evidenced by numerous high-quality publications, participation in prestigious scientific conferences with award-winning presentations, and invitations to numerous EU projects. It also participates in student education, collaborates with hospitals and physicians to test and implement new technologies, co-develops them further with the medical industry community, and fosters the creation of start-ups. Sano's work is strengthened by close collaboration with its Teaming partners: the University of Sheffield, FZ Jülich, Fraunhofer ISI, Cyfronet AGH, and the Klaster Lifescience Krakow.

The organisation of the Conference is the result of the experience gained during Sano Science Day (2023, 2024) and the Life Science Open Space events of the Krakow Klaster Lifescience (since 2019), as well as the extensive experience of the Faculty of Computer Science at AGH and the Academic Computer Centre Cyfronet AGH in this field. Given the organisers' expertise in high-performance computing, computer simulation, and artificial intelligence, the Conference will offer an excellent opportunity to foster greater interaction between communities working in the field of computational medicine.

Conference topics include

- Computational modelling of organs and diseases,
- Patient data management and processing,

- Analysis of medical images,
- Machine learning models for healthcare,
- Computer simulations using advanced computing infrastructures,
- Surgical planning tools,
- Model and simulation reproducibility and credibility,
- Clinical decision support systems based on artificial intelligence,
- Towards the Virtual Human Twin platform,
- Ethical, legal, and social issues in VHT.

The KCCM sessions are preceded by 6 tutorials prepared by the Sano and Cyfronet AGH teams, which aim to impart practical skills useful in broadly defined computational medicine. These also serve as a showcase of the practical competencies of Sano and Cyfronet teams.

The conference is divided into 7 sessions, each beginning with a keynote lecture. We are very grateful to renowned scientists: Ewa Deelman, Liesbet Geris, Tomasz Gosiewski, Alfons Hoekstra, Joanna Jaworek-Korjakowska, Emiliano Ricciardi, and Daniel Taylor for accepting the invitation to deliver these lectures and for their support of the Sano.

31 contributed papers from Sano, Faculty of Computer Science AGH, Cyfronet AGH, and collaborating institutions were accepted for presentation at the KCCM. They provide a very good overview of current research activity in computational medicine. We thank the authors of 10 papers for agreeing to present them as posters, which allowed us to avoid organising parallel sessions. The conference will conclude with a Summary session; we are convinced that it will be an inspiration to expand the research agendas of our three institutions with new, innovative research topics.

We are indebted to the members of the Steering, Program, and Organising Committees for their efforts aiming at preparing the best possible scientific meeting on computational medicine in Krakow. We owe thanks to the Mayor of the City of Krakow, Aleksander Miszalski, for granting honorary patronage to the Conference, as well as to the exceptional weekly magazine "Tygodnik Powszechny" for providing patronage to KCCM. This event is organised in the framework of the Sano Teaming project funded by the European Union's Horizon 2020 research and innovation program under grant agreement No 857533.

It's worth mentioning that there are currently 7 Teaming centres like Sano in Poland, dedicated to various domains of science, which draw on the best practices of their European partners in conducting and implementing research. These centres are unique and innovative elements in Polish science. Sano is the only such centre in Krakow and the Małopolska region, and is open to collaboration,

On behalf of the KCCM Steering Committee
Editors: Marian Bubak and Ewelina Szymańska-Skolimowska

Organization

KCCM 2025 was organized by:

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Faculty of Computer Science AGH

Academic Computer Centre Cyfronet AGH.

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Brain–Gut Axis and How to Study It

Jan K. Argasiński[1], Cemal Koba[1], Rosmary Blanco[1], Monika Pytlarz[1]

[1]Sano - Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland

{j.argasinski, c.koba, r.blanco, m.pytlarz} @sanoscience.org

Keywords: computational neuroscience, brain-gut axis, methodology, study design

1. Introduction

Compact binary mergers and the collapse of massive stars can produce intense transients obseThe brain–gut axis, a bidirectional communication network linking the central nervous system and the gastrointestinal tract, is emerging as a interesting domain in understanding neurological, metabolic, and psychiatric disorders. Despite growing biological and clinical interest, computational approaches to studying the brain–gut axis remain basic. This tutorial responds to the need for a methodological framework for researchers aiming to explore the brain–gut axis from a computational neuroscience perspective. Focusing on scientific literature as both a source of knowledge and a foundation for study design, the session will introduce participants to modern tools and strategies for initiating research in this field.

2. Description of the tutorial

This 3-hour tutorial serves as both a literature deep-dive and a methodology primer. Participants will work in a guided exploration of the latest scientific publications on the brain–gut axis, with a particular focus on computationally relevant research.

The session is divided into three components:

Literature Exploration and Mapping:

Participants will learn systematic methods for identifying, filtering, and categorizing relevant literature using tools like PubMed, Scopus, and AI-powered search engines (e.g., Semantic Scholar, Connected Papers). Emphasis will be placed on extracting methodological content, modeling approaches, and data sources.

Scientific Methodology for Study Planning:

We will demonstrate how to analyze existing studies to extract assumptions, computational models, and data modalities (EEG, fMRI, microbiome profiles, behavioral markers). Participants will collaboratively map gaps and research opportunities, developing hypotheses based on the current state of the field.

Pipeline Prototyping for Brain–Gut Studies:

The final part of the session will be a walkthrough of how to draft a computational research pipeline. This includes defining input data, identifying possible modeling techniques (e.g., neural networks, graph-based models, Bayesian inference), and conceptualizing evaluation strategies.

The goal is to help participants move from reading to research planning. The format includes short lectures, guided group work, and discussion.

3. Knowledge and skills to be gained

By the end of the tutorial, participants will be informed on how to:

- Conduct literature reviews focused on computational neuroscience topics.
- Identify and extract methodological insights from scientific publications.
- Recognize and categorize computational approaches applicable to brain–gut research.
- Formulate basic study designs for modeling the brain–gut axis.
- Draft conceptual pipelines for computational experiments, including data selection, modeling strategies, and analysis plans.
- Understand the interdisciplinary landscape of brain–gut research and the role of computational tools within it.

Acknowledgements. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857533 and from the International Research Agendas Programme of the Foundation for Polish Science No MAB PLUS/2019/13. The tutorial was created within the project of the Minister of Science and Higher Education „Support for the activity of Centers of Excellence established in Poland under Horizon 2020" on the basis of the contract number MEiN/2023/DIR/3796. We gratefully acknowledge Poland's high-performance Infrastructure PLGrid ACC Cyfronet AGH for providing computer facilities and support within computational grant no. PLG/2025/018289.

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CACTUS: Explainable AI for Knowledge Discovery and Classification

Jose Sousa[1]

[1]Sano - Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland

j.sausa@sanoscience.org

Keywords: explainable AI, data abstraction, knowledge graphs, classification, small datasets

1. Introduction

This Deep learning has achieved remarkable performance but often requires large datasets, s ignificant computer resources, and lacks transparency, making it hard to trust in sensitive fields such as healthcare and law. The Comprehensive Abstraction and Classification [1–4] Tool for Uncovering Structures (CACTUS) offers a transparent and efficient approach by:

- Supporting small and incomplete datasets,
- Preserving the semantic meaning of categorical variables,
- Building interpretable knowledge graphs for feature interactions,
- Providing feature ranking and community analysis for explainable classification,
- Offering memory-efficient, parallelised analysis.

2. Description of the tutorial

This 3-hour tutorial serves as both a literature deep-dive and a methodology primer. ParticipantsThis hands-on session introduces CACTUS for explainable AI and secure analytics. Participants will:

- Learn CACTUS architecture (decision tree, abstraction, correlation modules),
- Prepare datasets and YAML configs for flexible analysis,
- Abstract continuous and categorical features into interpretable forms,
- Generate and interpret knowledge graphs and feature rankings,
- Compare CACTUS with standard ML models on datasets like breast cancer, thyroid, heart disease, and its use on the allergies project.

3. Knowledge and skills to be gained

By the end of the tutorial, participants will be able:

- Understanding Explainable AI and CACTUS methodology,
- Running CACTUS for binary and multi-class tasks,
- for Visualising feature interactions with knowledge graphs,
- Interpreting feature rankings alongside decision trees and correlations,
- Applying best practices for incomplete or small datasets.

Acknowledgements. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857533 and from the International Research Agendas Programme of the Foundation for Polish Science No MAB PLUS/2019/13. The tutorial was created within the project of the Minister of Science and Higher Education "Support for the activity of Centres of Excellence established in Poland under Horizon 2020" on the basis based on contract number MEiN/2023/DIR/3796. We gratefully acknowledge Poland's high-performance Infrastructure, PLGrid ACC Cyfronet AGH , for providing computer facilities and support within the computational grant no. PLG/2025/018289.

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Your Journey to HPC and Beyond. A Guide to Research at Scale with the Model Execution Environment

Marek Kasztelnik[2], Piotr Nowakowski[1,2,] and Piotr Połeć[2]

[1]Sano - Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]ACC Cyfronet AGH, ul. Nawojki 11, 30-950 Kraków, Poland

p.nowakowski@sanoscience.org, {m.kasztelnik,p.polec}@cyfronet.pl

Keywords: modelling, simulation, HPC, SLURM, Model Execution Environment

1. Introduction

This tutorial provides an introduction to High-Performance Computing (HPC) and its application in scientific research. Participants will be guided through the fundamental concepts of HPC, learning how to leverage powerful computing resources for their research needs. The tutorial will feature the Model Execution Environment (MEE), a platform designed to simplify the execution of complex simulations and data analysis pipelines on HPC infrastructure. We will explore how MEE supports the integration and execution of scientific applications, drawing on real-world examples from European research projects.

2. Description of the tutorial

This 3-hour tutorial will be a blend of lectures and live demonstrations. The session will cover the following topics:

1. Introduction to HPC and the SLURM queuing system: We will begin with an overview of HPC concepts and a practical guide to using the SLURM workload manager for submitting and managing jobs on a cluster.

2. API-driven job submission: This segment will focus on programmatic job submission. Participants will learn how to use an API to submit jobs to the HPC cluster and how to integrate this functionality with an external web application.

3. Introduction to the Model Execution Environment (MEE): The final part of the tutorial will introduce the MEE. We will showcase how MEE streamlines the process of running scientific applications. This will involve:

    · an overview of how to define and manage complex computational workflows.

    · a case study from the InSilicoWorld project, demonstrating how MEE was used to store cohort data and run hundreds of simulations as part of a large-scale computational campaign. 3. Knowledge and skills to be gained

Upon completion of this tutorial, participants will be able to:

- Understand the fundamentals of High-Performance Computing,
- Submit and manage computational jobs on an HPC cluster using the SLURM scheduler,
- Programmatically submit jobs to an HPC cluster via an API,
- Understand the purpose and benefits of the Model Execution Environment (MEE).

Acknowledgements. This tutorial is made possible by the contributions and results from the following projects: EDITH (grant agreement no. 101083771), InSilicoWorld (grant agreement no. 101016503), GEMINI (grant agreement no. 101083771).

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Implementing Intelligence: Legal Challenges in Creating AI Solutions – a platform for sharing experiences

Wioletta Niwińska[1], Anna Kajda-Twardowska[1] and Michał Kosobudzki[1]

[1]Sano - Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland

{w.niwinska, a.kajda, m.kosobudzki}@sanoscience.org

Keywords: modelling, simulation, HPC, SLURM, Model Execution Environment

1. Introduction

Developing AI solutions requires not only technical expertise, but also careful legal and ethical considerations to protect the interests of creators, users, and companies. Adhering to the principles of trustworthy and responsible AI throughout the development process can determine a project's success . A broad, multidisciplinary perspective is key to developing AI systems that comply with normative principles, rules, and standards of trustworthiness.

2. Description of the tutorial

The workshop will last four hours and will include a presentation with moderated discussion and a practical session. The first part will provide participants with theoretical knowledge on AI project implementation, including legal frameworks, key concepts, and practical insights. The second part will focus on practical tasks designed to stimulate creative thinking, negotiation, and the application of acquired knowledge. Participants will work in groups and take on roles typically involved in AI projects to simulate decision-making processes and identify key legal and ethical considerations in AI implementation. The workshops will use various methods, including the Walt Disney method.

Open to all conference participants (minimum number of participants is 10) —from lawyers to developers, executives, and engineers—regardless of prior AI or legal experience. Bringing together participants from different professional backgrounds will help identify legal risks from various perspectives. The workshop will end with a group discussion and creation of "golden bullets" – key lessons and takeaways to consolidate new knowledge and skills.

3. Knowledge and skills to be gained

This workshop aims to increase awareness of the complex legal regulations surrounding AI, with a focus on intellectual property and data protection. Through this workshop, participants will gain tips on the information needed to verify and the steps worth planning when creating AI solutions.

Acknowledgements. This work is supported by the European Union's Horizon 2020 research and innovation program under grant agreement no. 857533.

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Virtual Reality for Medical Data Visualisation and Interaction

Przemysław Korzeniowki[1], Kuba Chrobociński[1,2], and Michał Motak[1]

[1]Sano - Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2] Division of Clinical Medicine, School of Medicine & Population Health, University of Sheffield, S1 2TN, Sheffield, United Kingdom

{p.korzeniowski, k.chrobocinski, m.motak}@sanoscience.org

Keywords: Virtual Reality, Medical Imaging, Visualisation, Data Interaction

1. Introduction

While Virtual and Augmented Reality (VR/AR) are widely recognised for their entertainment applications, their utility is rapidly expanding across diverse industries. Beyond popular uses in gaming, flight, and driving simulators, these technologies offer safe and cost-effective platforms for skill development and gaining practical insights. Immersive simulations, in particular, mitigate the risks and expenses associated with traditional training methods.

The medical field stands out as a particularly promising area for VR. Its applications range from psychology and surgery to comprehensive training programs. These demonstrate not only cost-effectiveness but also the ability to introduce novel elements that significantly enhance user perception and engagement.

2. Description of the tutorial

The tutorial will introduce basic concepts used for the development of interactive environments in Unity Game Engine for medical applications. DICOM images import and interaction are going to be presented. Example Virtual Reality environments will be explored, and their strong sides and limitations are going to be discussed. Surgical training simulators leveraging haptic devices will be presented.

3. Knowledge and skills to be gained

- Basic Unity Game Engine concepts
- Challenges associated with Virtual Reality for medical imaging
- Setting up a simple visualisation of a 3D image in VR using Unity Game Engine
- Usage of Surgical Simulators with Haptic Feedback

Acknowledgements. This work is supported by the European Union's Horizon 2020 research and innovation program under grant agreement no. 857533 (Sano) and the International Research Agendas program of the Foundation for Polish Science, co-financed by the European Union under the European Regional Development Fund.

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Scaling up your VVUQ Workflows. Practical Automation with EasyVVUQ and Dask on HPC.

Karol Zając[1], Piotr Nowakowski[1,2], and Levente Sandor[3]

[1]Sano - Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]ACC Cyfronet AGH, ul. Nawojki 11, 30-950 Kraków, Poland
[3] Department of Hydrodynamic Systems, Budapest University of Technology and Economics, Faculty of Mechanical Engineering, Műegyetem rkp. 3, H-1111 Budapest, Hungary

{k.zajac,p.nowakowski} @sanoscience.org, lsandor@hds.bme.hu

Keywords: VVUQ, Sensitivity Analysis, Workflow Automation, Large-Scale, HPC

1. Introduction

This tutorial introduces participants to modern tools for Verification, Validation, and Uncertainty Quantification (VVUQ) in scientific modeling, with a focus on automating and scaling VVUQ workflows on High-Performance Computing (HPC) infrastructure. Through the use of the EasyVVUQ library and Dask parallel computing framework, researchers can efficiently run complex Sensitivity Analysis (SA) and Uncertainty Quantification (UQ) campaigns across many simulations. The session aims to demonstrate how these tools integrate seamlessly with HPC schedulers such as SLURM and MPI environments, enabling robust, reproducible, and scalable VVUQ pipelines.

2. Description of the tutorial

The workshop will last four hours and will include a presentation with moderated discussion This 1-hour hands-on tutorial blends conceptual introduction with live demonstrations. It is designed for researchers and software engineers looking to adopt or streamline VVUQ methodologies in their computational workflows. The session will cover:

1. VVUQ Concepts and Motivation: Introduction to VVUQ in scientific computing.
2. Automating VVUQ with EasyVVUQ: Learn to define parameters, set up encoders/decoders, and run campaigns with EasyVVUQ.
3. Scalable Execution with Dask: Use Dask (JobQueue/MPI) with SLURM to distribute jobs and monitor performance.
4. Use Case: Hemodynamics Simulation Campaign (VirtualFD): Hands-on application to a real-world example from GEMINI project.

3. Knowledge and skills to be gained

By the end of this tutorial, participants will be able to:

- Understand the principles of VVUQ and their role in computational modeling.
- Set up and manage VVUQ workflows using EasyVVUQ.
- Configure and run large-scale UQ/SA simulations using EasyVVUQ and Dask
- Analyze and visualize sensitivity and uncertainty results efficiently.

Acknowledgements. This tutorial is made possible by the contributions and results from the following projects: InSilicoWorld (grant agreement no. 101016503), GEMINI (grant agreement no. 101083771).

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Keynote Speaker

Opportunities for AI in Modern Cyberinfrastructure: The Case of Scientific Workflow Management

Ewa Deelman

University of Southern California

deelman@isi.edu

Over the last two decades, scientific workflow management systems (WMSs) have enabled the execution of complex, multi-task applications on a variety of computational platforms, including today's exascale systems. They ensure efficient execution of computational and data management tasks, adhering to their data and control dependencies. During workflow execution, WMSs monitor the execution of tasks, detect anomalies and failures, and deploy recovery mechanisms when needed. If the workflow cannot be successfully executed, the WMS provides debugging information to help the scientist or cyberinfrastructure (CI) operator fix the problem. However, as workflows and CI grow in scale, heterogeneity, and complexity, traditional WMS approaches face challenges in scalability, adaptability and resilience.

Although research in WMS has explored a number of avenues from workflow composition using semantic technologies to resource provisioning, workflow scheduling, fault-tolerance, and provenance tracking, the methods employed were often heuristics-based and limited in their applicability. With semantic technologies, there was a significant amount of investment in the generation of appropriate ontologies that needed to happen in order to ease workflow composition. Today, AI technologies are making a significant impact on every aspect of our lives, and they are being used in science as well. Although they are also applicable to CI, potentially making it more performant and resilient, they have not yet made significant inroads. In this work, we focus on the exploration of the use of AI in the case of workflow management systems, exploring its use throughout the scientific workflow lifecycle from workflow design to workflow execution. We investigate the use of AI in the context of the existing Pegasus WMS, exploring embedding AI in current systems as well as reimaging workflow management to be fully distributed and resilient. This new model is inspired by enhanced swarm intelligence (SI), designed to dynamically adapt to failures and optimize the overall system.

The Pegasus WMS. Pegasus pioneered the use of planning in WMSs, enabling users to focus on their science by describing their workflows in a resource-independent way. Pegasus takes that description and automatically maps the jobs onto heterogeneous resources, determines the necessary data transfers between jobs, and optimizes the workflow for performance and reliability. The result is an executable workflow that includes compute job submit scripts and data management jobs for the target CI. Pegasus has a notion of the submit host from where the system submits jobs to multiple distributed resources within the CI ecosystem: HTC (high-throughput computing) and high-performance computing (HPC) resources, campus clusters, user-provisioned clouds, and the edge. Pegasus workflows are easy to compose using Python, Java, and R APIs as well as in Jupyter Notebooks, and are portable across heterogeneous CI.

PegasusAI: Integrating AI throughout the workflow lifecycle. Whereas Pegasus uses simple heuristics, PegasusAI, a new project started in 2025, explores a variety of AI technologies throughout the entire workflow lifecycle. For workflow composition, we are exploring retrieval-augmented generation, combining the generative capabilities of large language models (LLMs) with retrieval mechanisms, to support workflow discovery and composition by

providing context-specific suggestions that users can adapt as needed. Today, the user identifies or provisions the resources needed for execution. Once resources are provisioned, the WMS plans the workflow onto the resources using static heuristics. PegasusAI will fully automate the resource provisioning and planning steps. The planner will identify the types of resources needed, and then the provisioner will acquire the needed resources before the planner maps the workflow onto them. To make smart decisions, we explore a variety of AI models, including neural network-based models and probabilistic models, to learn about resource and job performance and robustness. Once the workflow is sent for execution, PegasusAI monitors the jobs in real time and performs anomaly and error detection (slow network, overloaded system, application error) using techniques such as Graph Neural Networks, LLMs, or autoencoders that we explored in prior work and decide whether to adapt the execution or the mapping or suggest to the user to modify the workflow. As results are being generated, PegasusAI learns about successful workflow design patterns and their components.

Part of the challenge of adopting AI for CI may be the quick pace of AI development as well as the challenges associated with the deployment of the technologies. Overtime, one needs to have a way of migrating between AI models as the new generations become more capable. This includes the evaluation of new technologies in terms of the validity of the solution, performance, and resource needs, as well as potential additional fine-tuning, "catching up" with the latest model to what the previous version already learned about the CI context. Issues of deployment, such as availability of appropriate computational and storage resources over time to support learning and inferencing, issues of resilience when models are embedded in the CI, or connectivity when queried remotely, need to be taken into account.

SWARM: Scientific Workflow Applications on Resilient Metasystem. Pegasus and PegasusAI are designed to be production-level capabilities. Pegasus is being used today in astronomy, bioinformatics, climate and weather modeling, ecology, earthquake science, gravitational-wave physics, materials science, chemistry, and AI/ML for science. PegasusAI will build on the current capabilities and incrementally incorporate AI to make the system easier to use, more performant, and robust. However, there are limitations to the current approach, as the system is centralized. SWARM, on the other hand, reimagines the WMS as fully distributed and agentic, making agents responsible for the distributed compute resources across the computing continuum, from the edge to the core.

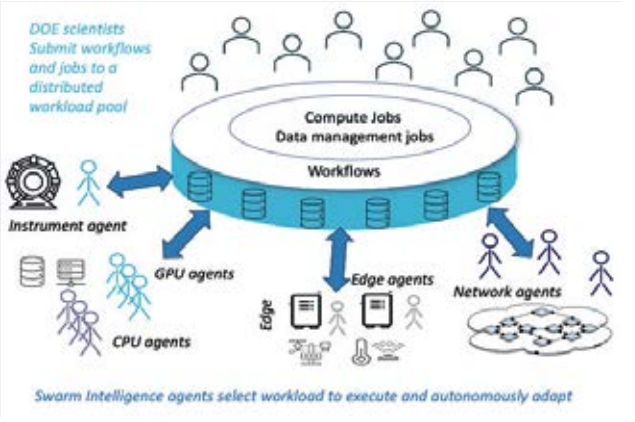

Fig. 1. Overwiew of the SWARM System.

SWARM integrates swarm intelligence, consensus protocols, and optimized network over-

lays. Instead of relying on a centralized scheduler, SWARM models job scheduling, data management, and fault recovery as autonomous yet cooperative agents—ranging from lightweight edge agents to LLM-enhanced cognitive agents—that self-monitor, diagnose, and adapt to failures. Consensus plays a central role: heterogeneous agents achieve agreement on job selection and resource allocation using tailored consensus functions and resilient algorithms, such as Practical Byzantine Fault Tolerance and novel greedy variants, which ensure progress even under failures. To address scalability and efficiency, SWARM employs dynamic overlay networks, where the communication topology adapts to resource capabilities and network conditions, balancing local and global connectivity to minimize overhead while maintaining robustness. The multi-agent work includes a fault-tolerant, fully distributed scheduling architecture that eliminates the single points of failure common in centralized systems. Independent agents manage local resources, monitor system health, and coordinate through competitive bidding, achieving near-optimal job allocation without heavy consensus overhead. SWARN is meant to be a research effort that explores ideas of agentic AI for CI. However, we expect that some of the ideas will be valuable in production.

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Keynote Speaker

Building the Virtual Human Twin: from an engaged ecosystem to an incipient infrastructure

Liesbet Geris

University of Liège, KU Leuven & VPH Institute

liesbet.geris@kuleuven.be

Following the definition of the European Commission, a Virtual -Human Twin (VHT) is a digital representation of a human health or disease state. VHTs refer to different levels of human anatomy (e.g. cells, tissues, organs or organ systems). They are built using software models and data and are designed to mimic and predict behaviour of their physical counterparts, including interaction with additional diseases a person may have. The key potential in health and care of this technology is related to targeted prevention, tailored clinical pathways, and to supporting healthcare professionals in virtual environments. Examples include implementation of clinical trials for medicines and devices, medical training, surgical intervention planning, and several other potential use cases in virtual world environments. A public VHT infrastructure is the subject of an ongoing tender. This infrastructure should enable the pooling of resources and assets (data, models, algorithms, computing power, storage etc.) to develop these twins in healthcare and assess their credibility. Hence, it should entail the development of a federated public infrastructure and the collection of said resources, driven by the engagement of a collaborative ecosystem.

In order to realise the potential of the VHT, a shared vision and inclusive eco-system driven roadmap has been developed, supported through the EDITH Coordination and Support Action. The roadmap contains a blueprint of the Virtual Human Twin and will identify the required (technical) developments, including but not limited to interoperability, computability, hardware and integration of health models & data. Ethical, Legal and Social elements are discussed, including privacy, intellectual property rights, standards, regulations, ethics and social acceptance. The user perspective is developed for a range of stakeholders, whose needs and value propositions have been identified through a range of activities and interactions. Finally, sustainability of the ecosystem and infrastructure are examined, looking at incorporation in clinical and industrial workflow, development of economic activities, a member-state strategy and the creation of a public research infrastructure organisation. Recommendations for all involved stakeholders have been formulated. The final draft of the roadmap can be found here: https://zenodo.org/records/14645647.

In this talk I will discuss the current status and challenges that lie ahead on the road to realization of the vision of the Virtual Human Twin, using examples of my own research group as well as the work of colleagues.

Keynote Speaker

The digestive tract microbiome – where does it come from, how does it change, and what is its connection with the brain?

Tomasz Gosiewski

Jagiellonian University Medical College

tomasz.gosiewski@uj.edu.pl

Microbiome it is a mysterious phenomenon that is talked about and written about in the media. Often mistakenly referred to as flora or microflora, but it has nothing to do with plants. So what is the microbiome? It is a large collection of genes of microorganisms that inhabit their host and usually do not harm it, but on the contrary, cooperate with it. Sometimes another term also appears, namely microbiota. The microbiota is nothing more than all the cells or viruses that inhabit their host. So why two separate terms, the microbiome and the microbiota? Because by using research methods based on genetic analysis, we study the genes of microorganisms, i.e. the microbiome, and by detecting individual cells of microorganisms directly, we describe the microbiota. However, genetic studies provide a more comprehensive understanding of our microscopic neighbours, so they are preferred by scientists.

We acquire the microbiome at birth, because this is when the newborn has "first contact" with microorganisms, although some believe that this happens while still in the womb. What this contact will be like depends on the type of birth, and the optimal one is the natural one. As it passes through the birth canal, the newborn and its digestive tract are colonized by bacteria that inhabit the vagina, which are the beginning of the normal microbiome. If the mother feeds the newborn with her own milk, she additionally supports the developing microbiome. Delivery by caesarean section causes bacteria from the hospital environment (pathogenic, multidrug-resistant) to enter the newborn's digestive tract first and they initiate the microbiome (abnormal). The microbiome profile in the first days and weeks of life determines the likelihood of developing inflammatory diseases later in life. An abnormal gut microbiome increases the risk of diseases such as diabetes, obesity, inflammatory bowel disease, allergies, autoimmune diseases, autism, and many others.

Is the microbiome related to the brain? It is surprising, but scientific discoveries indicate that it is. The composition of the gut microbiota influences the dense network of neuronal connections that wraps around the gut. Neurons produce neurotransmitters such as serotonin, norepinephrine, dopamine and others. The microbiota influences the chemical profiles of neurotransmitters in the gut, which in turn transported through the blood to the brain and affect it. On the other hand, the brain, through the vagus nerve, influences intestinal peristalsis and, therefore, the microbiota. These interactions are being studied intensively and are an exciting field for neuroscience and neuropsychoatrics.

Keynote Speaker

Towards Digital Twins for Cerebral Blood Flow and Perfusion Pathologies

Alfons Hoekstra

University of Amsterdam

a.g.hoekstra@uva.nl

A multiscale computational model for for cerebral blood flow, perfusion, and tissue metabolism will be introduced. The main components are: (1) a 0D blood flow model including the heart, large systemic arteries, the Circle of Willis, and smaller cerebral arteries projecting on the pial surface; (2) a 3D brain perfusion model using a three-compartmental porous medium approach capturing the length scales of the arterial, capillary, and venule vessels of the brain; and (3) a tissue metabolism and tissue death model. Details of the components and their couplings will be discussed, as wel as validation results. Two examples of digital twin using these computational models will be introduced: (1) estimation of infarcts in acute ischemic stroke patients (using the fully coupled model); (2) estimation of orthostatic hypotension in elderly individuals (only relying on the 0D blood flow component).

Keynote Speaker

Artificial Intelligence in Orthodontics: From Automated Diagnostics to Personalized Treatment

Joanna Jaworek-Korjakowska

AGH University

jaworek@agh.edu.pl

Artificial intelligence (AI) is increasingly transforming orthodontics by enabling more precise diagnostics, treatment planning, and patient monitoring. Machine learning algorithms applied to radiographs, 3D scans, and intraoral images can automatically detect anatomical landmarks, classify malocclusions, and predict treatment outcomes with high accuracy. Deep learning models facilitate automated cephalometric analysis, reducing human error and saving clinical time. In addition, AI-powered simulation tools allow for individualized treatment planning, such as predicting tooth movement and optimizing aligner design. Beyond diagnostics and planning, AI supports remote monitoring through image-based progress tracking, enhancing patient engagement and enabling timely interventions. Ethical and clinical considerations, including data privacy, bias, and explainability, remain central to integrating AI safely into practice. Overall, AI offers significant potential to improve efficiency, accuracy, and personalization in orthodontic care, paving the way for more accessible and patient-centered treatments.

Keynote Speaker

Modeling the Sensory-Deprived Brain: Insights from Neuroimaging, Computational Neuroscience, and Machine Learning

Emiliano Ricciardi

IMT School for Advanced Studies Lucca

emiliano.ricciardi@imtlucca.it

How does the brain adapt to the absence of an entire sensory modality from birth? This question has long fascinated neuroscientists interested in the balance between neural plasticity and biological constraints. In this talk, I will present recent efforts from our group at the IMT School for Advanced Studies Lucca, where we integrate high-resolution neuroimaging and machine learning approaches to explore how the brain reorganizes itself under conditions of congenital sensory deprivation.

Combining techniques such as multivariate pattern analysis, machine learning approaches and functional network modeling to neuroimaging data, we describe how distributed brain networks reorganize and how conceptual knowledge emerges independently of visual input. We then feed these neural signals into deep generative models, allowing us to reconstruct high-level visual representations from brain activity in congenitally blind individuals.

These interdisciplinary approaches reveal a dual nature of cortical organization: a stable, hierarchically structured architecture that persists without sensory input, and a flexible layer of experience-driven reallocation. By bridging empirical and computational neuroscience, our work contributes to a deeper understanding of how the human brain maintains functional integrity and cognitive richness even in the face of profound sensory absence.

Keynote Speaker

Computing coronary physiology: Conception, Optimisation and Clinical application

Daniel Taylor

University of Sheffield

daniel.taylor@sheffield.ac.uk

Computed coronary physiology (virtual FFR) is now established in clinical practice. Our group recently developed a model for predicting absolute flow and hyperaemic coronary microvascular resistance using pressure wire and angiographic data. In this talk I will first outline how we developed the model and implemented side branch flow. I will then cover the optimisation and validation of these advancements. Finally, I will discuss how the model may be used to enhance clinical practice, by applying it retrospectively to data from the landmark ORBITA trial. Specifically, I will explore the relationship between disordered coronary microvasculature and the symptomatic response to percutaneous coronary intervention in patients with stable angina.

Poster

Development of a Diagnostic Decision-Support System for Allergic Diseases at the Voivodeship Rehabilitation Hospital for Children in Ameryka

Paulina Tworek[1], Maja Szczypka[1,2], Marek Mikołajczyk[3], Roman Lewandowski[3,4], Jose Sousa[1]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2] Institute of Computer Science, AGH University of Krakow, A. Mickiewicza 30, 30-059, Krakow, Poland
[3] Voivodeship Rehabilitation Hospital for Children in Ameryka, Ameryka 21,11-015, Poland
[4] Institute of Management and Quality Sciences, Faculty of Economics, University of Warmia and Mazury, Oczapowskiego 13, 10-719 Olsztyn, Poland

{p.tworek, m.szczypka, j.sousa}@anoscience.org,
m.mikołajczyk@ameryka.com.pl, roman.lewandowski@uwm.edu.pl

Keywords: classification, allergies, decision support system, explainable-AI, real-world implementation

1. Introduction

The rapid digitalization of healthcare presents new opportunities to enhance clinical outcomes [1]. Allergic diseases affect up to 35% of children and are steadily increasing worldwide [2]. Their development involves multiple factors, leading to highly diverse symptoms and making diagnosis difficult. Challenges include the wide range of allergens, the role of cofactors, inconsistent test correlations, and the absence of fully standardized diagnostic protocols adapted to different medical examinations and age groups [3]. As a result, effective control of allergic diseases is still difficult. While both AI and medicine continue to progress rapidly, the integration of AI-based decision-support tools in hospital practice faces significant challenges, including incomplete datasets, variability in laboratory methods, and the absence of unified diagnostic standards. Moreover, transparency remains a critical requirement: diagnostic algorithms must provide explanations that are understandable to both clinicians and patients.

2. Description of the problem

Although both AI and medicine are advancing quickly, the adoption of AI-driven decision support tools in clinical practice is hindered by major challenges such as incomplete datasets, inconsistencies in procedures, and the lack of standardized diagnostic criteria [4]. Yet many existing approaches, particularly deep learning models, still lack the interpretability needed for safe and reliable clinical application. A major challenge is the development of a system capable of analyzing noisy data with many missing values while maintaining explainability of the results. It is also essential to integrate structured and unstructured types of data.

3. Related work

Allergic diseases present considerable complexity, as they are characterized by diverse clinical manifestations and heterogeneous pathogenic pathways. This multifaceted nature poses challenges for establishing a reliable diagnosis. Several solutions have been proposed in the field of allergic diseases: tools designed to support asthma management, monitoring applications or mobile apps designed to help doctors assess adverse drug reactions in terms of causality, severity, and preventability [5, 6, 7]. Although many systems are being developed, they often focus mainly on functionalities related to health process management rather than directly supporting the diagnostic process. Furthemore, they are frequently designed or tested on very small patient

groups, limiting their generalizability.

4. Solution to the problem

To address the previously mentioned challenges faced by clinical decision support systems, the Comprehensive Abstraction and Classification Tool for Uncovering Structures (CACTUS) was developed. It was decided to implement this system at the Allergy Department at the Voivodeship Rehabilitation Hospital for Children in Ameryka. The dataset obtained from the hospital consisted of medical test results as well as interviews with nurses and physicians. Test-related information was provided in tabular form. Each patient was diagnosed and assigned to one of International Classification of Diseases (ICD-10).

The aim was to assess CACTUS performance in a real-world clinical setting and to examine its ability to enhance diagnostic procedures and assist healthcare professionals. It is important to note that CACTUS operates on tabular data. However, a significant amount of crucial information in hospitals is stored in unstructured form, which made it necessary to extract data from text and integrate it with data obtained from medical examinations. Information extraction was performed using two distinct approaches: rule-based techniques and large language models (LLMs). A classification process was conducted using CACTUS to identify allergic disease types. The obtained classification results and stability of key features were compared with those of classic machine learning classification methods.

5. Conclusions

The conducted real-world experiment demonstrates the promising role of CACTUS as a decision-support system for diagnosing allergic diseases. CACTUS achieved high classification accuracy compared to traditional methods. In addition, the experiments highlighted its stability, which is essential not only for increasing physicians' trust in the system but also for improving clinical efficiency by identifying and omitting examinations that are not diagnostically meaningful. Future work will focus on extracting additional information from physicians' and nurses' interviews, which can further strengthen the classification process. Another important direction of development will be the creation of a multi-agent system.

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Poster

Interpretable Machine Learning for Glioma Grading from HLA-DR–Stained Whole-Slide Images: Multi-Feature Analysis with SHAP

Monika Pytlarz[1], Yevgheni Petkevich[1], Kamil Wojnicki[2], Beata Kaza[3], Wiesława Grajkowska[4], Łukasz Michałowski[5], Bożena Kamińska[3], Jan Argasiński[1]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]University Children's Hospital Zurich, Lenggstrasse 30, 8008 Zürich, Switzerland
[3]Nencki Institute of Experimental Biology, 3 Pasteur Street, 02-093 Warszawa, Poland
[4]Department of Pathology, The Children's Memorial Health Institute, Av. Dzieci Polskich 20, 04-730 Warsaw Poland
[5]Department of Pathology, University Clinical Centre of the Medical University of Warsaw, Jana Nielubowicza 5, 02-097 Warszawa, Poland

{m.pytlarz, y.petkevich, j.argasinski}@sanoscience.org, kamil.wojnicki@kispi.uzh.ch, {b.kaza, b.kaminska}@nencki.edu.pl, w.grajkowska@ipczd.pl, michalowski.patologia@gmail.com

Keywords: glioma; interpretable classification, microglia/macrophages; HLA-DR/DP/DQ; digital pathology; amoeboid vs ramified; Cellpose, image complexity; radiomics

1. Introduction

Computer-assisted intervention (CAI) is a research field focused on enhancing the safeGliomas show heterogeneous histomorphology and immune infiltration that correlate with tumor grade. Microglia/macrophages, identified by HLA-DR, adopt morphologies ranging from ramified to amoeboid, reflecting activation states. Manual assessment of whole slide images (WSIs) is laborious and subjective, creating a need for automated and interpretable grading approaches.

2. Description of the problem

Computational histopathology of glioma WSIs faces biological heterogeneity, technical variability, and the requirement of model transparency. As AI for medical imaging moves beyond opaque black-box models [1,2], reproducible approaches linking predictions to underlying biology are required to support clinical adoption.

3. Related work

Activated microglia/macrophages shift from ramified to amoeboid morphology and are more common in higher grades [3–5]. Beyond cell features, image-complexity measures can reflect tumor heterogeneity and may relate to IDH mutation status [6]. Recent studies reflect a growing interest in explainable approaches to glioblastoma assessment [2], yet immune-related features have been less frequently investigated in computational histopathology, despite evidence of their prognostic relevance.

4. Solution to the problem

We developed an interpretable ML pipeline for HLA-DR–stained WSIs (WHO G1–G4) with robust preprocessing, integrating immune morphology, image complexity, and deep features. Interpretability was ensured through SHAP, linking predictions to underlying biology. The dataset comprised 110 HLA-DR/DP/DQ–stained glioma WSIs, tiled into 1024×1024 px patches with 10% overlap, with background removed using conservative HSV-based subtraction. Nuclei

were segmented with a pretrained Cellpose [7] model; HLA-DR-positive cytoplasmic/membranous signal was segmented using HSV thresholding and assigned to nuclei via watershed, yielding cell-level morphology descriptors. We then extracted 4 feature categories (Fig. 1): (1) morphology (ramified vs amoeboid phenotypes), (2) image complexity (e.g., entropy, fractal dimension, lacunarity), (3) radiomics (first- and second-order), and (4) deep embeddings (ResNet-50). Preliminary classification used XGBoost with SHAP. Entropy rose prominently from G2 to G4, with G4 showing the highest values and greatest variability, indicative of increased heterogeneity. The amoeboid fraction rose with grade. XGBoost reached 0.93. SHAP ranked entropy as the top feature, with ResNet-50 embeddings, first-order radiomics, and amoeboid count also in the top five.

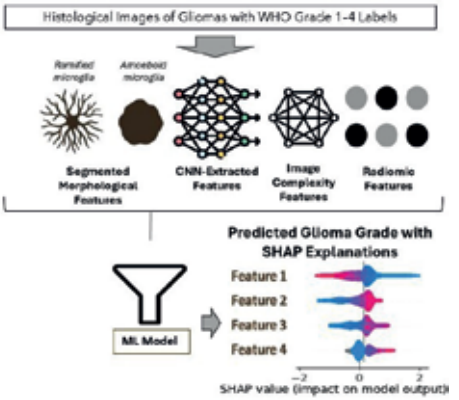

Fig. 1. Pipeline design.

5. Conclusions and future work

SimuScope successfully generates realistic, diverse, and semantically consistent synthetic surgical images from a lightweight training process using only 100 frames of real data. It achieves a high mean Intersection over Union (mIoU) of 70.65%, confirming excellent preservation of semantic labels. While the Fréchet Inception Distance (FID) is slightly higher than the baseline, the Kernel Inception Distance (KID) of 0.0690 is comparable and acceptable, showing a strong balance between realism and label fidelity. The use of ControlNet is crucial for enhancing texture and color. The main limitation is the lack of temporal coherency between frames; future work will aim to address this by focusing on video-to-video generation.

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Poster

Application of Deep Learning to Quantify Brain Microstructure

Dominika Ciupek[1], Maciej Malawski[1,2], Tomasz Pięciak[3,1]

[1] Sano Centre for Computational Medicine, Kraków, 30-054 Poland
[2] AGH University of Kraków, Kraków, 30-059 Poland
[3] ETSI Telecomunicación, Universidad de Valladolid, Valladolid, 47011 Spain

{d.ciupek, m.malawski}@sanoscience.org, tpieciak@tel.uva.es

Keywords: diffusion-weighted magnetic resonance imaging, multicompartment models, deep learning

1. Introduction

Diffusion-weighted magnetic resonance imaging (DW MRI) offers valuable insights into cellular structures, making it a powerful tool for the non-invasive evaluation of brain microstructure. This modality is particularly sensitive to natural processes of brain maturation and aging, and various neurological disorders [1]. However, accurate modeling of the DW signal is crucial for extracting quantitative indicators, especially when the acquisition procedure is limited.

2. Description of the problem

Diffusion tensor imaging (DTI) [2] is a widely used technique for modeling the DW signal, but interpreting its data can be challenging as it only captures the primary direction of diffusion [1]. An alternative approach involves using multicompartment biophysical models that assume specific tissue geometries and can directly estimate key microstructural parameters, making data interpretation easier [3]. Two of the most popular biophysical models are Neurite Orientation Dispersion and Density Imaging (NODDI) [4] and the Spherical Mean Technique (SMT) [5] (see Fig.1). Microstructural parameters derived from multicompartment models are typically calculated using numerical optimization procedures. However, these methods require more complex and time-consuming acquisition protocols, including a specific number of DW volumes, than those commonly used in clinical practice. This complexity significantly limits the practical application of biophysical models in clinical settings.

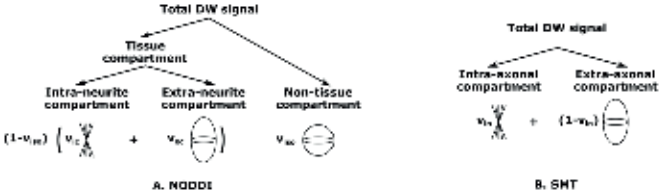

Fig. 1. Distribution of the total DW signal between different compartments of the A. NODDI and B. SMT models.

3. Related work

Research in the literature has explored the potential application of deep learning to estimate parameters of multicompartment models, especially the NODDI [6,7]. However, these studies are quite limited in scope. They often focus only on the effects of a reduced number of DW volumes, while employing acquisition schemes that are not commonly used in clinical practice.

4. Solution to the problem

The study utilized the HCP WU-Minn data [8], which originally included 90 gradient directions for three b-values (1000, 2000, and 3000 s/mm2). To simulate acquisition protocols

more representative of clinical settings [9], the data were downsampled and interpolated using spherical harmonics to generate three separate datasets with b = 1000 s/mm² and 32, 15, and 6 gradient directions. Microstructural parameters were estimated using both traditional numerical optimization techniques and a deep learning-based U-net model. Parameters derived from the original, full-resolution acquisition were used as the ground truth for comparison. Performance evaluation was conducted using the Mean Structural Similarity Index Measure (MSSIM). A summary of the results is provided in Table 1.

Tab. 1. MSSIM results of the U-Net and a standard numerical method across different acquisition schemes, assessed for various parameters of the SMT and NODDI models.

	32 volumes, b1000		15 volumes, b1000		6 volumes, b1000	
Microstructural parameter	DL model	Numerical method	DL model	Numerical method	DL model	Numerical method
v_{ic}	0.950	0.703	0.947	0.704	0.945	0.698
v_{ec}	0.785	0.099	0.791	0.103	0.784	0.116
v_{iso}	0.884	0.484	0.887	0.488	0.867	0.495
v_{in}	0.833	0.225	0.823	0.218	0.823	0.065

5. Conclusions and future work

Deep learning models significantly outperform traditional numerical method, achieving MSSIM values over 0.8 for all parameters except vec, even with only 6 gradient directions. To better assess ability of artificial intelligence to estimate microstructural parameters, we should move beyond U-Net to more advanced models like GANs, and focus on metrics more clinically relevant than MSSIM, particularly in key regions of the brain. It's also crucial to determine if these models can effectively differentiate parameter values between healthy individuals and those with diseases to support accurate diagnosis.

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Poster

Beyond Accuracy: Assessing the Impact of EEG Denoising on the Diagnostic Utility of a Pre-Hospital Stroke Triage Model

Rosmary Blanco[1], Jan K. Argasiński[1], Maritta N. van Stigt[2], Eva E. Groenendijk[2], Jonathan M. Coutinho[2], Aneta Lisowska[3], Henk A. Marquering[2]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Department of Neurology, Department of Radiology and Nuclear Medicine / Biomedical Engineering and Physics, Amsterdam University Medical Center, location University of Amsterdam, Meibergdreef 9, 1105 AZ Amsterdam, the Netherlands
[3]Vrije Universiteit / Amsterdam University Medical Center, location University of Amsterdam, Meibergdreef 9, 1105 AZ Amsterdam, the Netherlands

{r.blanco, j.argasinski}@sanoscience.org, {m.n.vanstigt, e.a.groenendijk, j.coutinho, a.j.lisowska, h.a.marquering}@amsterdamumc.nl

Keywords: EEG, AutoML, Artifact Removal, Stroke

1. Introduction

Rapid and accurate diagnosis of acute stroke is essential for improving patient outcomes; however, distinguishing stroke from stroke mimics in pre-hospital settings remains a major clinical challenge [1]. Machine learning (ML) techniques have shown promise in early, data-driven stroke prediction [2]. Electroencephalography (EEG) offers a portable, non-invasive tool for assessing brain function, but its diagnostic utility depends critically on robust signal processing to mitigate noise and artifacts [3]. This study assesses how automated EEG artifact removal methods affect ML model performance, reliability, and classification errors in differentiating ischemic stroke, hemorrhagic stroke, and stroke mimics.

2. Description of the problem

Low-density EEG systems with dry electrodes are well-suited for real-world clinical applications because of their portability and rapid setup. However, they are more prone to large, non-stereotypical artifacts, resulting in a low signal-to-noise ratio. Traditional artifact removal methods require expert intervention, making them impractical for real-time or time-sensitive applications [4]. Evaluating EEG denoising is challenging due to the lack of a clean ground-truth signal. Most studies assess efficacy via downstream task performance (e.g., classification accuracy) [5], but this may overlook effects on diagnostic reliability and clinical safety. Automated pipelines are needed to preserve diagnostically relevant neural features under real-world conditions.

3. Related work

Prior research has established the value of quantitative EEG features as biomarkers of cerebral ischemia and has increasingly leveraged ML to automate stroke detection [6]. However, most pioneering studies rely on a single, pre-defined denoising pipeline [7]. A systematic comparison of how alternative preprocessing strategies influence the clinical utility and error profile of diagnostic models, particularly for low-density EEG, remains a significant gap in the literature [8].

4. Solution to the problem

We analyzed data from 719 patients from the prospective, multicenter ELECTRA-STRO-

KE and AI-STROKE studies, including 389 ischemic strokes and 330 non-ischemic cases (stroke mimics and hemorrhagic strokes). For each patient, 2–3 minutes of resting-state EEG were recorded using a portable 8-channel dry-electrode system. We compared five artifact removal methods: Wavelet Transform (W), Empirical Mode Decomposition (EMD), Artifact Subspace Reconstruction (ASR), and two hybrid approaches, ASR-W and EMD_W [9], against a minimally processed (filtered) baseline. Each dataset was independently processed with AutoML (AutoPrognosis) [10] to identify the optimal ML pipeline, which optimized the AUROC in a 5-fold cross-validation scheme for unbiased comparison. Final performance was assessed on a held-out test set using AUROC, the DeLong test for statistical comparison, and clinical error analysis, including diagnosis-specific misclassification patterns and clustering of error profiles. Comparative analysis revealed that denoising choice influenced diagnostic value, beyond standard accuracy metrics. The EMD-W pipeline achieved the highest AUROC (0.938), not significantly different from the minimally processed baseline (0.930; $p = 0.678$). ASR-W performed significantly worse (0.908; $p = 0.049$). Crucially, error profile analysis showed that EMD-W reduced missed strokes to 15, compared with 20 in the baseline and 31 with ASR. In contrast, ASR_W accumulated the most errors (56), misclassifying largely stroke mimics such as TIA and "Other" cases. These findings highlight a trade-off: advanced denoising does not always improve overall predictive accuracy but can critically impact diagnostic safety.

5. Conclusions and future work

Evaluation of preprocessing pipelines should go beyond accuracy metrics, and it is advisable to test multiple denoising methods to identify the approach that maximizes diagnostic utility and ensures model safety. This work represents a foundational step toward building reliable, data-driven physiological models for virtual human twin platforms, demonstrating that rigorous, automated processing is essential to translate noisy, real-world EEG data into clinically trustworthy solutions.

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Poster

Sharp-to-Soft CT Kernel Conversion Using Quaternion and Variational Decomposition Mode

Mahmoud Nasr[1,2], Krzysztof Brzostowski[3], and Adam Piórkowski[2]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Department of Biocybernetics and Biomedical Engineering, AGH University of Krakow, Poland
[3]Wroclaw University of Science and Technology, Faculty of Information and Communication Technology, Wroclaw, Poland.

m.nasr@sanoscience.org

Keywords: CT, Kernel Conversion, Quaternion, Bilateral Filter, VMD, Image Denoising

1. Introduction

Computed tomography (CT) imaging is fundamental to contemporary diagnostic radiology, and image quality is significantly affected by the reconstruction kernel. Sharp kernels improve edge clarity but generate considerable noise, whereas soft kernels diminish noise at the expense of obscuring small features. Transforming images from sharp to soft kernels is crucial for uniform image analysis and subsequent tasks such as segmentation or radiomics, eliminating the need for further scans. Recent studies have investigated deep learning and filtering-based methodologies to tackle this difficulty [1, 2].

2. Description of the problem

The main difficulty is to reduce the noise in sharp-kernel CT images while maintaining structural information to align with soft-kernel reconstructions. Conventional filters may blur edges or inadequately attenuate noise. Deep learning methodologies yield superior conversion quality, but need significant computer resources and extensive training datasets, restricting their practical application in clinical environments. An effective method for converting sharp kernel images to soft-like images, without significant data requirements or feature loss, is greatly sought after.

3. Related work

The previous studies have investigated both model-based and learning-based methodologies for CT kernel conversion and denoising. Deep convolutional networks have shown proficiency in transforming sharp- kernel images into soft-kernel counterparts while preserving structural details. However, they require considerable training data [1]. Based filtering methods provide an alternative by simulating the point spread function of the scanner to facilitate kernel conversion [3]. Sparse representation methods have been suggested for CT denoising, efficiently diminishing noise while maintaining image structures. Although effective, these methods require extensive datasets or prior knowledge of the system parameters, underscoring the need for a practical and efficient solution.

4. Solution to the problem

We offer an innovative kernel conversion framework that amalgamates bilateral quaternion filtering (QBF) [4] with decomposition methodologies, such as Variational Mode Decomposition (VMD) [5]. Our method in Fig. 1 utilizes a quaternion representation of CT images to process multichannel information, maintaining interchannel correlations concurrently. QBF efficiently diminishes noise and sharpens edges, generating soft-kernel images from sharp-kernel

inputs. Compared to deep learning techniques, our methodology requires limited data and processing duration, which makes it highly appropriate for therapeutic applications.

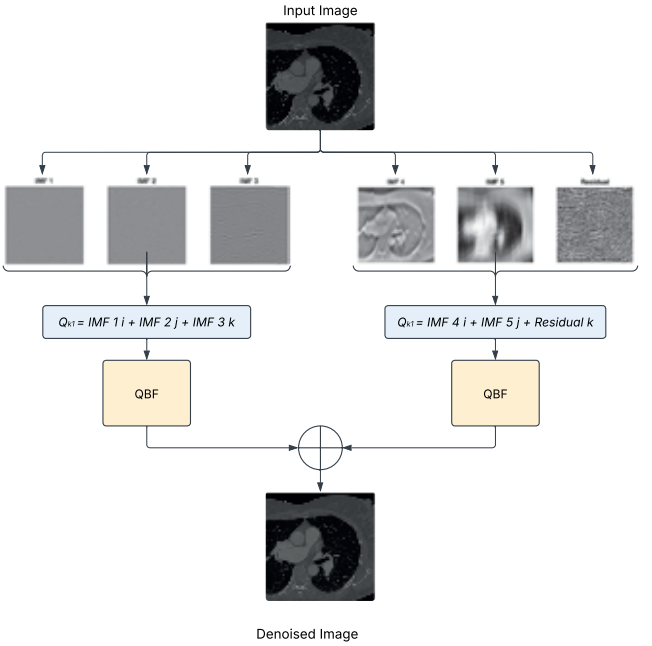

Fig. 1. The Proposed Method for representing the VMD IMFs to Quaternion form and Applying the QBF.

5. Conclusions and future work

SimuScope successfully generates realistic, diverse, and semantically consistent synthetic surgiThe suggested quaternion-based technique offers a practical and pragmatic solution for CT kernel conversion, producing soft-kernel-like images from sharp-kernel inputs while maintaining structural integrity and minimizing noise. This paradigm diminishes reliance on extensive training datasets and expedites processing time relative to deep learning techniques. Subsequent efforts will concentrate on incorporating this methodology into automated segmentation processes and assessing its generalizability across multi-center datasets.

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Poster

Realistic Endoscopic Synthetic Dataset Generation Through Surgical Simulation and Diffusion Models

Sabina Martyniak[1], Joanna Kaleta[1,2], Diego Dall'Alba[1,3], Szymon Płotka[1,4], Przemysław Korzeniowski[1]

[1]Sano Centre for Computational Medicine, [2]Warsaw University of Technology
[3]University of Verona, [4]University of Warsaw

s.martyniak@sanoscience.org

Keywords: Diffusion Models, surgical simulation, Synthetic Data Generation

1. Introduction

Computer-assisted intervention (CAI) is a research field focused on enhancing the safety, efficiency, and cost-effectiveness of medical procedures by minimizing errors and complications [1]. Within CAI, Laparoscopic Cholecystectomy (LC) has gained significant attention [2]. However, LC presents technical challenges due to limited visibility and the use of laparoscopic instruments, leading to potential complications like bile duct injury (BDI) [3]. To address these issues, generating synthetic data is a promising solution, but bridging the domain gap between synthetic and real data remains a challenge. We propose SimuScope, a pipeline that requires minimal real data, preserves annotation integrity, and has the potential to support the development of robust DL models for surgical assistance.

2. Description of the problem

To address these complexities, CAI systems leveraging Deep Learning (DL) methods have been proposed. These systems rely on deep learning models trained on complex and difficult-to-annotate data. Generating synthetic data is a promising solution, but bridging the domain gap between synthetic and real data remains a challenge.

3. Related work

Recently, several approaches have been proposed for generating synthetic data with realistic characteristics. While GAN-based approaches show potential, they have limitations, such as early convergence of discriminators and instability of adversarial training, leading to mode collapse and reduced diversity in generated data [4]. Diffusion models (DMs) [5] emerge as a promising alternative, surpassing GANs in computer vision tasks. Although multiple generative works exist in the medical and surgical fields, a gap remains in surgical data generation, particularly for fully labeled simulator-based data with accurate and detailed instrument-tissue interactions [6,8]. Based on simulation data, [6] generates large fully labeled realistic endoscopic images, addressing the minimal data requirement. However, this work also relies on a very simple simulator lacking tool-tissue interactions.

4. Solution to the problem

We use a custom simulator built in Unity3D integrated with an XPBD (Extended Position--Based Dynamics) solver implemented in C/C++. This allows real-time soft-tissue simulation with grasping, cutting, clipping, tearing, and thermo-coagulation. Anatomical models include liver, gallbladder, cystic duct and artery, simulated as tetrahedral meshes. Our method involves

adding a new style to the SD model and using it to generate realistic images from synthetic ones. We begin by fine-tuning SD based on LoRA [7]. Then, the fine-tuned Laparoscopic Cholecystectomy Stable Diffusion model is employed to generate realistic images. For realistic tissue generation, we use text-guided image-to-image inference with additional control. The input to the model is raw simulator image. The proposed method is depicted in (Fig. 1).

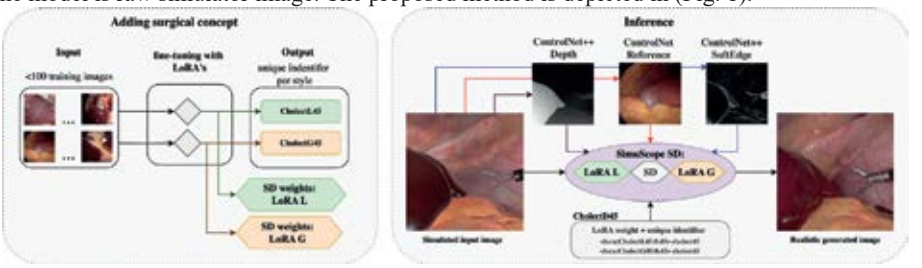

Fig. 1. SimuScope uses a Stable Diffusion model, fine-tuned with LoRA and conditioned by ControlNet, to generate realistic surgical images from simulator input.

5. Conclusions and future work

SimuScope successfully generates realistic, diverse, and semantically consistent synthetic surgical images from a lightweight training process using only 100 frames of real data. It achieves a high mean Intersection over Union (mIoU) of 70.65%, confirming excellent preservation of semantic labels. While the Fréchet Inception Distance (FID) is slightly higher than the baseline, the Kernel Inception Distance (KID) of 0.0690 is comparable and acceptable, showing a strong balance between realism and label fidelity. The use of ControlNet is crucial for enhancing texture and color. The main limitation is the lack of temporal coherency between frames; future work will aim to address this by focusing on video-to-video generation.

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Poster

Dynamic Profiling of the Sinonasal Microbiome Using Nanopore Sequencing in the Diagnosis of Chronic Rhinosinusitis

Sylwia Bożek[1], Tomasz Kościółek[1], Joanna Szaleniec[2]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Department of Otolaryngology, Faculty of Medicine, Jagiellonian University Medical College, Kraków, Poland

{s.bozek,t.kosciolek}@sanoscience.org, joanna.szaleniec@uj.edu.pl

Keywords: microbiome, antibiotic resistance, bioinformatics, rhinosinusitis, full-length 16S rRNA sequencing, nanopore, longitudinal analysis, personalized medicine

1. Introduction

The sinonasal microbiome is a complex community of microorganisms. In Poland, standard diagnosis for chronic rhinosinusitis primarily relies on microbiological cultures, which are often insufficient for detecting the full spectrum of microorganisms. In response to these challenges, the dynamic development of modern molecular techniques, including third-generation sequencing and long-read technologies, enables profiling the microbiome with species-level precision.

2. Description of the problem

Many bacteria don't grow in standard culture conditions or grow very slowly, which can lead to an incomplete diagnosis. By comparing data obtained through sequencing with the results of classic cultures, it's possible to identify discrepancies, complementary information, and detect clinically significant patterns that remain invisible in standard diagnostic practice. Additionally, understanding the dynamics of human-associated microbial communities allows us to track changes in the microbiome in response to internal factors (e.g., health status) and external factors (e.g., treatment, environment). As recent studies have shown, sampling from a single site may not be universally representative of the entire sinus microbiome due to significant spatial variability [1]. In this study, we use full-length 16S rRNA gene sequencing with Oxford Nanopore Technologies, which allows for microorganism identification with species-level resolution.

3. Related work

Prior research on the sinonasal microbiome has predominantly utilized short-read sequencing, limiting the taxonomic resolution of microorganism identification to the genus level.

Third-generation nanopore sequencing enables species-level microbial community profiling [2]. In the sinuses, species-level differentiation is particularly important because microorganisms from the same genus can exhibit extremely different behavior. For example, Staphylococcus aureus has a wide variety of proinflammatory virulence factors, and its presence is related to refractory rhinosinusitis while Staphylococcus epidermidis is supposedly a commensal that may protect from S. aureus colonization [3-5].

4. Solution to the problem

To address the limitations of traditional diagnostic methods and single time-point analyses, our study focuses on the advanced analysis of long-read data. Because Oxford Nanopore Technology is characterized by a higher error rate than other sequencing methods, we use the

PRONAME pipeline [6] for data processing. This pipeline integrates quality and length filtering, clustering, and advanced error correction to produce high-quality consensus sequences. We also use the precompiled Greengenes2 database [7], which enables precise species-level taxonomic classification. The processed microbiome data is then analyzed for changes over time to detect patterns and trends that are invisible in single time-point analyses. Our approach not only allows for longitudinal microbiome profiling but also enables a direct comparison with the results of classical microbiological cultures. This confrontation provides information about bacteria that don't grow in laboratory conditions and may play a significant role in disease pathogenesis. By comparing sequencing and culture data, we verify the accuracy and sensitivity of both methods, revealing how full-length 16S rRNA gene sequencing can provide a much more complete picture of the microbiome and detect potentially overlooked microorganisms.

5. Conclusions and future work

Our analysis of the current study group has shown that the composition of the sinonasal microbiome in patients with chronic rhinosinusitis and in healthy individuals does not show consistent patterns but is instead highly individual. In the future, we plan to expand the study group. This will allow us to continue our longitudinal analyses and thoroughly investigate temporal trends in the microbiome's composition. Additionally, we aim to evaluate the impact of systemic antibiotic therapy on the sinonasal microbiome, including changes in its taxonomic composition and the presence of antibiotic-resistant bacteria. In the long term, we will seek to integrate microbiome data with other clinical data. This is crucial for creating a patient's digital twin and applying personalized medicine in routine clinical practice.

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Poster

Aggregating gut: on the link between neurodegeneration and bacterial functional amyloids

Alicja W. Wojciechowska[1,2], Jakub W. Wojciechowski[1], Kinga Zielinska[3], Johannes Soeding[4], Tomasz Kosciolek[1], Malgorzata Kotulska[2]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Wroclaw University of Science and Technology, Faculty of Fundamental Problems of Technology, Department of Biomedical Engineering, Wroclaw, Poland
[3]Malopolska Centre of Biotechnology, Jagiellonian University, Krakow, Poland
[4]Max Planck Institute for Multidisciplinary Sciences, Gottingen, Germany

{a.wojeciechowska, j.wojciechowski, t.kosciolek}@sanoscience.org, kinga.zielinska@uj.edu.pl, soeding@mpinat.mpg.de, malgorzata.kotulska@pwr.edu.pl

Keywords: microbiome, neurodegeneration, protein

1. Introduction

The human gut microbiome is known to influence human health by providing essential substances and modulating immune responses. The onset and progression of neurodegenerative diseases are dependent on these processes, though the details of the gut-brain crosstalk in these disorders remain elusive. Recent studies reveal that gut bacteria produce bacterial functional amyloids, proteins with structures similar to the misfolded human proteins linked to neurodegenerative diseases [1]. This structural similarity allows them to potentially trigger or accelerate the aggregation of human proteins, such as alpha-synuclein, a key protein in Parkinson's disease [2]. This process may originate in the gut and spread to the brain via the vagus nerve, suggesting that the disease could start in the gut [2, 3]. Further research is necessary to fully understand the role of these bacterial amyloids, which could lead to new diagnostic and therapeutic strategies for neurodegenerative diseases.

2. Description of the problem

To fully understand the role of bacterial functional amyloids in neurodegeneration, we must investigate three key areas. First, we are interested in estimating how many such proteins are produced by the human gut microbiome. Second, we want to evaluate whether the abundance of such proteins is associated with the disease. Finally, we aim to identify human molecular pathways which could be affected by bacterial functional amyloids.

3. Related work

Wang et al. [4] have shown that E. coli bacterial amyloid CsgA promotes neuropathologies by inducing the aggregation of pathological amyloids, colocalizing with them in the neurons and downregulating the mitochondrial genes in C. elegans. Intestinal Bap amyloids produced by Staphylococcus have been found to promote neurodegeneration in mice and proposed as future biomarkers of such pathologies [5].

4. Solution to the problem

Using a bioinformatics approach, we identify gut microbiome functional amyloids and analyze their potential impact on human health via the gut-brain axis. The results point to taxonomically diverse sources of functional amyloids (Fig. 1) and their frequent presence in the

extracellular space. The retrieved interactions between gut microbiome functional amyloids and human proteins indicate their potential to trigger inflammation, affect transport and signalling processes. We also find a greater relative abundance of bacterial functional amyloids in patients diagnosed with Parkinson's disease and specifically a higher content of the curli amyloid protein, CsgA, in Alzheimer's disease patients than in healthy controls.

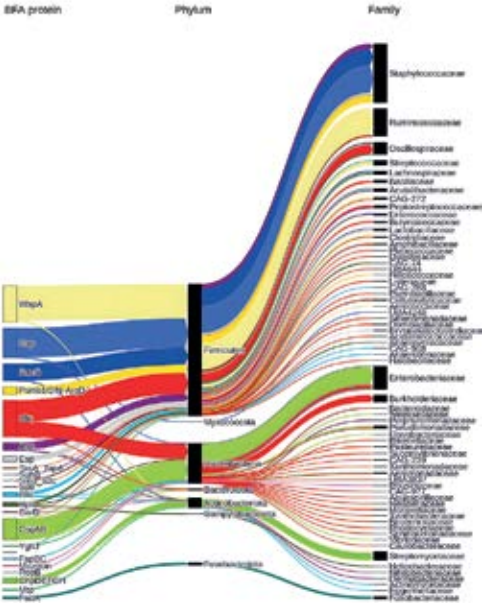

Fig. 1. Taxonomic distribution of bacterial functional amyloids found in the human gut microbiome proteome.

5. Conclusions and future work

Our results provide a rationale for the tentative link between neurodegeneration and gut bacterial functional amyloids. The future research could focus on the potential of bacterial functional amyloids as biomarkers in these disorders. The preprint is available at: https://www.biorxiv.org/content/10.1101/2024.11.26.624671v1.

Acknowledgements. We acknowledge the support of EU under grants EDITH No 101083771 (Digital Europe), GEMINI No 101136438 (HORIZON), Meetween No 101135798 (HORIZON), and Teaming Sano No 857533. This work was supported by the National Science Centre, Poland [2019/35/B/NZ2/03997] (MK) and NAWA STER grant of Polish National Agency for Academic Exchange for PhD students (JWW). TK is funded by the National Science Centre, Poland [2023/05/Y/NZ2/00080]. We would like to cordially thank Prof. Pawel P. Łabaj for valuable comments.

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Towards Trustworthy Digital Twins in Healthcare: VVUQ Activities in the GEMINI Project

Karol Zając[1], Piotr Nowakowski[1,2], Marek Kasztelnik[2], Piotr Połeć[2], Marian Bubak[1,2]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Academic Computer Centre Cyfronet AGH, Nawojki 11, Krakow, Poland

{k.zajac,p.nowakowski,m.bubak}@sanoscience.org,{m.kasztelnik,p.polec}@cyfronet.pl

Keywords: Digital Twin, VVUQ, Personalized Healthcare, Modelling and Simulation, HPC

1. Introduction

Digital twins hold great promise for transforming modern healthcare by enabling predictive, individualized simulations that inform diagnosis and treatment. In this context, the GEMINI project [1] aims to create a new generation of multi-scale digital twins for patients suffering from ischemic and hemorrhagic stroke. A critical pillar of the project is ensuring the reliability and credibility of these digital models, particularly in clinical settings where robust decisions depend on model quality.

2. Description of the problem

While high-fidelity models exist for various physiological systems, their translation into digital twin systems requires rigorous testing to guarantee validity. In complex simulations, errors can arise from numerical methods, parameter uncertainty, or model assumptions. The Verification, Validation, and Uncertainty Quantification (VVUQ) [2] processes are therefore essential for assessing model credibility and quantifying confidence in their predictions, especially when models influence therapeutic decisions.

3. Related work

The need for systematic VVUQ processes is increasingly recognized within the digital twin community, including in projects like In Silico World [3] or EDITH [4]. However, many existing pipelines still struggle with scalability and reproducibility, especially when faced with new use cases or when applied to large patient cohorts and HPC environments. Sano, in GEMINI, aims to bridge this gap by integrating modular and scalable VVUQ workflows directly into its simulation framework.

4. Solution to the problem

As part of the project, Sano leads a dedicated effort to design and implement a VVUQ methodology aligned with the overall GEMINI digital twin pipeline. This includes:

- Implementation of automation tools (e.g., EasyVVUQ [5] and Dask [6]) for running large-scale uncertainty and sensitivity analyses [Fig.3].
- Integration with HPC platforms (via SLURM, MPI, Dask) for scalable deployment across thousands of simulations [Fig.2].
- Tracking and storing simulation metadata, reproducibility, and versioning (Model Execution Environment [7]) [Fig.1]. to comply with future certification standards.

Multiple generic execution solutions have been proposed to manage simulation runs across multiple models and patient cohorts, supporting reproducible VVUQ experimentation.

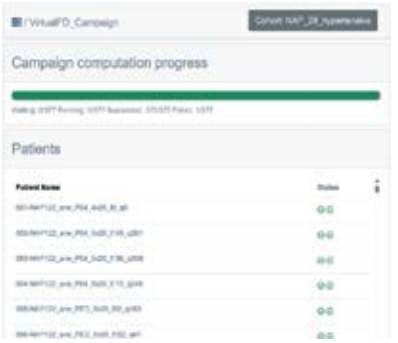

Fig. 1. MEE campaign management view for a cohort of patients.

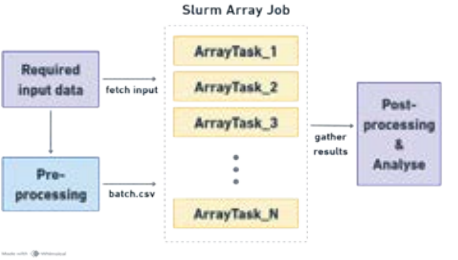

Fig.2. Massively parallel study diagram using SLURM array job.

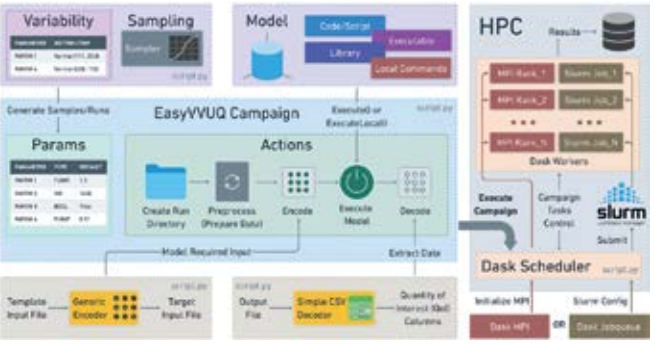

Fig. 3. General workflow diagram for UQ/SA experiments using EasyVVUQ and Dask.

5. Conclusions and future work

Sano's work in GEMINI lays the foundation for trustworthy and certifiable medical digital twins. By embedding reproducible VVUQ workflows into the digital twin lifecycle and validating them on stroke-related models, we contribute a critical building block for future clinical adoption. The next steps involve tighter integration with clinical and data partners, further automation, and simulation workflow optimization.

Acknowledgements. We acknowledge the support of EU under grants GEMINI No. 101136438, as well as ACC Cyfronet AGH for providing computer facilities and support within computational grant No. PLG/2024/017108 and PLG/2025/018168.

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Poster

Research Data Sharing Incentivisation Toolkit

Taras Zhyhulin[1], Karol Zając[1], Marek Kasztelnik[2], Maciej Malawski[1,2], Jan Meizner[1,2], Piotr Nowakowski[1,2], Piotr Połeć[2]

[1] Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2] Academic Computer Center Cyfronet AGH, Nawojki 11 Street, 30-950 Krakow, Poland
*Authors contributed equally

{t.zhyhulin,k.zajac.,m.malawski,j.meizner,p.nowakowski}@sanoscience.org,
{m.kasztelnik,p.polec}@cyfronet.pl

Keywords: data sharing, FAIR principles, Dataverse, RODBUK, HPC

1. Introduction

Data sharing plays a crucial role in the modern scientific community, as it can significantly reduce research costs and improve the quality of future related studies. To encourage scientists to share their data, the process must be simplified and made more convenient through the development and implementation of user-friendly tools. Additionally, providing incentives can further motivate researchers to engage in data sharing.

2. Description of the problem

Medical simulations require large volumes of input and output data, which must be securely stored and easily accessed by research teams. Without standardised, user-friendly infrastructure, researchers risk data loss, duplication, and security breaches. These simulations also demand a lot of computational power, requiring secure data transfer to external environments such as HPC.

Although data-sharing tools exist, researchers often lack integrated workflows that connect storage, collaboration, and execution. This fragmentation hinders reproducibility and discourages data sharing. Incentives for collaboration and reuse remain limited, further contributing to data loss.

Additionally, to increase citation and reuse potential, data must be properly disseminated. Therefore, a seamless, secure, and incentivised data sharing framework tailored to computational medicine is urgently needed.

3. Related work

This work is motivated by the 2009 findings of Paul Glasziou and Iain Chalmers, who reported that around 85% of reusable research data is lost due to being unpublished or poorly documented [2]. This highlights the need for structured data sharing and preservation, especially in data-intensive fields like computational medicine.

The Galaxy Project [3] offers an integrated platform for data storage, computation, and analysis across disciplines. However, its general-purpose design makes it less suited to the specific demands of medical simulations, where data sensitivity and workflow complexity require a more focused, domain-specific approach.

4. Solution to the problem

We deployed an institutional Dataverse instance, named Sano Dataverse [4], providing a secure and user-friendly platform for internal data sharing and convenient publication.

To improve visibility, credibility, and security, Sano joined RODBUK – a Polish federation of Dataverse instances. It enforces advanced security policies, aggregates datasets in a central portal for better discoverability, and holds CoreTrustSeal certification, ensuring FAIR compliance and long-term preservation.

To streamline data transfer between storage and HPC environments, we integrated the Model Execution Environment platform [5] with Dataverse, Zenodo, and InvenioRDM. This enables an end-to-end workflow: retrieving data, processing it in HPC, and uploading results back.

We also developed a rule-based data sharing strategy, illustrated by the DPValid [6] dataset on Sano Dataverse. It incentivises users to contribute related data post-publication, supporting ongoing dataset growth. The strategy uses built-in repository features and aligns with the integration framework.

Fig.1. Toolkit for enhanced data sharing and collaboration.

5. Conclusions and future work

The developed solutions – Sano Dataverse as part of the RODBUK federation, the integration between the Model Execution Environment (MEE) and data repositories such as Dataverse, Zenodo, and InvenioRDM, as well as the implementation of a rule-based data sharing strategy – collectively form a toolkit that simplifies the data sharing process and encourages researchers to make their data available. Furthermore, it is in line with Open Science and FAIR principles, supporting the broader shift toward collaboration and data reuse in the scientific community.

Acknowledgements. This publication is partly supported by the EU H2020 grants Sano (857533), ISW (101016503) and by the Minister of Science and Higher Education „Support for the activity of Centers of Excellence established in Poland under Horizon 2020" number MEiN/2023/DIR/3796. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017022.

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Oral presentation

Augmenting not replacing: preparing the future health workforce for the digital tools revolution in clinical reasoning

Andrzej A. Kononowicz[1*], Joanna Fąferek[2], Ada Frankowska[1], Anna Kocurek[2], Małgorzata Sudacka[2], Renata Szydlak[1]

[1]Department of Bioinformatics and Telemedicine, Jagiellonian University Medical College, Medyczna 7, 30-688 Kraków, Poland
[2]Center for Innovative Medical Education, Jagiellonian University Medical College, Medyczna 7, 30-688 Kraków, Poland

{andrzej.kononowicz, joanna.faferek, ada.frankowska, anna.kocurek, malgorzata.sudacka, renata.szydlak}@uj.edu.pl

** on behalf of the D-CREDO project consortium*

Keywords: clinical reasoning, digital health tools, clinical decision support systems, virtual patients

1. Introduction

Clinical reasoning (CR) is the cognitive skill health professionals use in practice to observe, collect, and analyze information in order to diagnose and manage patients, taking into account their specific circumstances and preferences [1]. Poor CR performance directly contributes to medical errors and must continually be improved to ensure a safe and efficient healthcare system. A wide range of digital tools are currently available to enhance CR in practice.

2. Description of the problem

Despite the excellent performance of many digital tools in simulated, individual CR tasks, their integration in clinical practice faces significant challenges. For instance, it has been observed that human-machine collaboration does not necessarily lead to improvements in practice and, in some cases, artificial intelligence (AI) alone performs better than when used in collaboration with humans [2]. One explanation is the limited proficiency in using the technology. Consequently, methods are being sought to redesign medical education in order to prepare future health professionals to use emerging technologies efficiently as synergistic partners in CR.

3. Related work

Several CR curricula and methods to support the acquisition of this skill are available [3-5]. Researchers have also proposed general approaches to learning CR in alignment with digital tools [1,2]. However, what remains lacking is a comprehensive curriculum with learning resources that explicitly address the use of digital tools in CR.

4. Solution to the problem

The D-CREDO project [6], a three-year initiative launched in 2024 and funded by the European Commission, aim to develop a curriculum that teaches both undergraduate health professional students and their teachers how to use digital tools in CR practice. The authors, representing the coordinating institution, work closely with project partners from Austria, Germany, the Netherlands, and Ukraine across several stages of the curriculum development process. The needs analysis comprised 30 semi-structured interviews and 118 survey responses collected across partner institutions. It enabled the selection of digital tool categories considered particularly relevant for the CR process: AI in image analysis, large language models and big data

technologies, mHealth applications and wearables, electronic health records with clinical decision support functionality, and telehealth technologies such as videoconferencing and remote monitoring. Building on a systematic rapid review of more than 1500 abstracts from the literature [7] and a Delphi consensus process with associated partners, the consortium has developed a catalogue of 26 learning objectives and produced a white paper outlining selected learning and assessment strategies, both available as deliverables on the project website: https://d-credo.eu. At the current stage, the project is finalizing a blueprint of more than ten new learning units that extend the existing DID-ACT curriculum [4]. The curriculum is grounded in theoretical frameworks such as distributed cognition theory, cognitive load theory, and experiential learning theory, and is designed to include a range of self-directed and group learning activities. This activities will cover, e.g. CR-focused prompt engineering techniques, role-played virtual visits, strategic data synthesis of patient information across the electronic health record, and the ethical and legal aspects of CR with digital tools. The learning units will feature virtual patients adapted from the iCoViP repository, illustrating the use of D-CREDO digital tools in CR practice [5].

5. Conclusions and future work

During the first year, the D-CREDO project delivered a comprehensive set of source materials, along with an understanding of the needs of the stakeholders involved in CR education. These will be transformed into interactive learning units based on the blueprint during the second year of the project, and then verified and refined in the final year based on eight implementation studies. The associated partner network of the project is open to collaboration with external institutions interested in adopting the learning units or contributing digital tools relevant for CR practice and education. Such tools can be integrated into the curriculum as examples, and thereby learned, tested, and disseminated by a broader community of future health professionals.

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Oral presentation

LLM-based psychological digital twins in social research: opportunities and dangers

Paweł Sobkowicz[1,2]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Narodowe Centrum Badań Jądrowych, , ul. A Sołtana 7, 04-500 Otwock-Świerk, Poland

p.sobkowicz@sanoscience.org, pawelsobko@gmail.com

Keywords: Agent Based Models, ABM, LLM, digital twins, DT

1. Introduction

We discuss here the potential benefits of using LLM engines in social and psychological studies, in particular as a component of coordinated experimental/simulation projects. The advances in LLMs – particularly those trained on general corpora of human generated texts taken from social life – offer a novel opportunity, creating agents that can be defined and tested using normal language.

2. Description of the problem

Agent Based Models(ABMs) have been used in studies of social phenomena for over 55 years. They range from extremely simplistic (where humans are described through a single binary variable (for example in opinion dynamics studies using tools and analogies with the Ising model of magnetism) to more complex approaches, where an agent is characterized by multiple variables, has complex internal rules determining its actions and reactions (goals, preferences, memory), and acts in complex social environment. Despite progress in computing power, these complex models are quite rare. There are several reasons for this. First, human psychology is very complex, and there is no dominant "theory of foundations human behavior", on which modelers could build their simulation frameworks. Second, the experimental data, necessary to derive and validate the rules determining agent behaviors is fragmented (most of social and psychological studies are not designed with the goal of providing data to facilitate creation of ABMs). Third, such rule-based model is only as good as the completeness of variables and rules sets are, and as the starting conditions correspond to actual situations.

3. A different approach to the problem

In recent years, a new approach has appeared: use of LLMs to create agents (or even agent societies), corresponding to desired psycho-social characteristics ("generative agents models"). The agents are defined through dedicated prompts, and may be "asked" to perform actions, react to situations in a way that corresponds to the predefined profile. This allows simulations to correspond closely to real world situations. The advances in general purpose LLMs since 2024 have resulted in a veritable explosion of the published papers, conference presentations and preprints devoted to uses of such generative agents (for reviews, see e.g [1-3]). At the same time, the nascent field has definite weaknesses and problems [4-7]. We shall discuss potential benefits and limitations of the above approach using simple, illustrative examples (based on imaginary personal descriptions). They show, that while the potential promise of the generative ABMs is great, the current state of the art requires careful validation.

4. Challenges, conclusions and future work

There are two types of challenges facing generative agents' approach. The first is technical: how to ensure the "independence" and stability of personas created using LLMs. Today's LLMs still leave a lot to improve. Also, while it is relatively easy to program individual agents or very small groups, simulations of large communities requires new tools and untested scalability.

But far more important are ethical challenges. By their very definition, successful psychological digital twins can "reproduce" behavioral characteristics of specific people. This opens way to myriad of possible abuses, some relatively mild (using a DT for marketing/advertising choice purposes), to very dangerous, like political manipulation. Thus, special care should be present in planning research devoted to the topic and in development of the associated tools.

At the same time, the ease with which we can map real world situations into simulations and obtain understandable results is tempting. However, to fulfill the promise of such DT/generative agents, they must be verifies and validates – by comparing them with experiments and with the rule-based ABMs (where the mechanisms are known by definition). Optimally, the LLM-based approach might serve as an improvement engine for traditional models, by discovering the rules of behavior hidden in the LLM structures.

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Oral presentation

Personalizing Dyslexia Interventions with a Virtual Cognitive Twin Framework

Suvarna Rekha Chinta

Jagiellonian University, Romana Ingardina 6, Krakow, Poland

suvarna.rekha.11@gmail.com

Keywords: Virtual Human Twin (VHT), Cognitive Twin, Simulation-based prediction, Multimodal data integration, Precision intervention, Dyslexia

1. Introduction

The concept of the Virtual Human Twin (VHT) has primarily focused on physiological and biomedical modelling to advance personalized medicine [2][5]. However, cognitive and neurodevelopmental disorders such as dyslexia and other developmental disorders remain underrepresented in this framework, despite their high prevalence and lifelong impact on education, mental health, and social functioning. Integrating multimodal cognitive and behavioral markers into VHT can expand its scope, enabling more inclusive and personalized supporting and rehabilitative solutions.

2. Description of the problem

Current dyslexia research has produced valuable datasets on eye movements, rapid automatized naming, phonological awareness, attentional control, and psychophysiological responses. But these modalities are analyzed in isolation, limiting their predictive value and clinical applicability. There is no fixed computational framework that integrates these heterogeneous markers into a unified model that can simulate, predict, and personalize dyslexia remedial outcomes within the VHT paradigm.

3. Related work

Digital twin approaches in medicine are demonstrating the utility of multiscale modelling for organs and diseases (e.g., the Virtual Physiological Human initiative) [4]. Recent computational psychiatry studies also suggest disorder-specific learning signatures in dyslexia and ADHD, supporting the feasibility of latent-state modelling [1][3]. However, no existing studies have systematically adapted such approaches to dyslexia in a way that could feed into VHT platforms.

4. Solution to the problem

We propose a preliminary framework for a Virtual Cognitive Twin for dyslexia. Using our dataset of dyslexic and typical readers, including eye-tracking, electrodermal activity (EDA), phonological awareness, and attentional network test (ANT) data, we outline a multimodal integration pipeline. First, features are extracted from each modality to capture cognitive and physiological signatures. Next, machine learning classifiers are applied to identify markers of dyslexic vs. typical reading profiles. Finally, the outputs are conceptualized as latent parameters (e.g., processing efficiency, attentional control, phonological mapping) that could be embedded into a computational model simulating individual reading behavior. This approach provides a demonstrator level contribution to the VHT ecosystem by extending modelling to cognition and learning disorders.

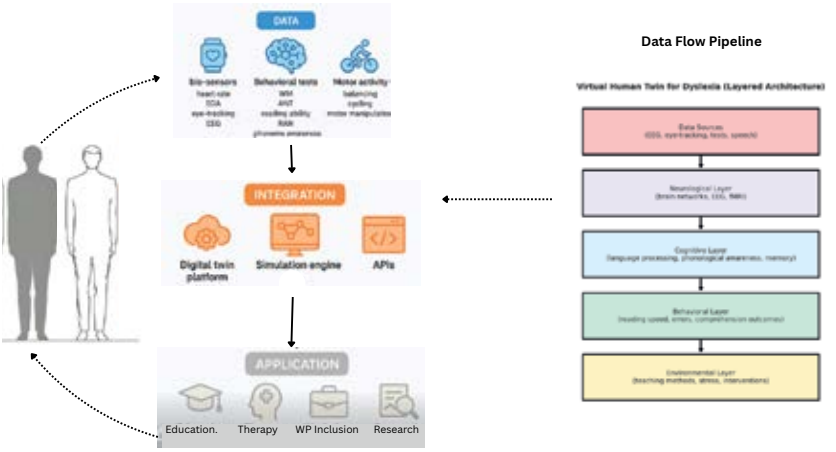

Figure 1. Conceptual architecture of the proposed Virtual Cognitive Twin for dyslexia, integrating attentional, physiological, and language related markers into a simulation engine for individualized prediction and intervention support.

5. Conclusions and future work

This work represents an initial step towards incorporating neurocognitive disorders into the Virtual Human Twin paradigm. By integrating multimodal markers of dyslexia into a unified model, we move closer to a platform that not only captures psychophysiology but also cognitive function. Future work will expand datasets, refine classifiers, and test clinical populations, ultimately contributing to personalized intervention strategies for dyslexia and related disorders within the VHT framework.

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Oral presentation

On-Device Radiotherapy Simulation: Secure Computing in Your Browser

Konrad Michalik, Łukasz Kwinta, Leszek Grzanka

Akademia Górniczo-Hutnicza, al. Mickiewicza 30, 30-059 Kraków, Poland

{kmichalikk,lukasz.kwinta}@student.agh.edu.pl, grzanka@agh.edu.pl

Keywords: HPC, medical simulations, radiotherapy, particle transport simulations

1. Introduction

In computational medicine, particle transport simulations are essential for advancing radiotherapy treatment planning, especially in X-ray and proton therapy. While commercial Treatment Planning Systems (TPS) provide fast dose calculations, Monte Carlo (MC) methods deliver a more detailed description of particle interactions. Beyond dose, MC simulations compute quantities such as Linear Energy Transfer (LET) and energy spectra, which are critical in hadrontherapy for assessing biological effects. Elevated LET can improve tumor control but is also linked to late toxicities such as brain lesions and necrosis, particularly in patients treated for brain, head-and-neck, ocular, or prostate tumors. Because of these risks and the need for precise biological modeling, MC simulations serve not only as a research tool but also as a benchmark for validating TPS algorithms. Geant4 [1] is the most widely used toolkit for these applications, yet its practical use often requires significant technical expertise. Even GUI-based solutions remain complex and combined with the need to handle sensitive patient data, this creates notable challenges in accessibility and security.

2. Description of the problem

Monte Carlo particle transport simulations like Geant4 face challenges limiting their adoption in computational medicine, especially dosimetry in radiation therapy. Geant4 is a programming library requiring users to build custom applications, demanding programming skills and command-line knowledge, which narrows its user base. Traditional setups involve complex installations and dependencies, often requiring Linux expertise, creating barriers for many clinicians and researchers. HPC or cloud-based solutions overcome this barrier but create different ones - handling sensitive patient data risks breaches and regulatory issues when transferred to external servers. Modern web technologies offer a solution by enabling serverless, browser-based simulations that run locally, eliminating software installation and protecting sensitive data through on-device processing.

3. Related work

Several efforts have focused on porting Geant4 to WebAssembly for browser-based simulations. Guy Barrand demonstrated feasibility by porting Geant4 examples and an ESS accelerator simulator with live preview, though without full input editing or sharing. A CERN Google Summer of Code project also explored this, showing viable simulation and visualization performance in WebAssembly. The OHIF Viewer highlights secure, on-device processing of medical imaging in browsers, preserving privacy by avoiding server uploads, demonstrating accessible and confidential healthcare tools [2]. Additionally, research shows AI and medical simulations can run efficiently in browsers using WebAssembly and WebWorkers, enabling parallel, high-performance client-side computation.

4. Solution to the problem

We propose a preliminary framework for a Virtual Cognitive Twin for dyslexia. Using our dataseOur project provides a web-based platform for Monte Carlo particle transport simulations running entirely on-device within web browsers. By compiling Geant4 to WebAssembly with Emscripten, we enable secure, server-free simulations on user hardware. This browser-compatible Geant4 version runs sandboxed and leverages multi-core CPUs via WebWorkers for improved parallel performance. Dynamic data management allows on-demand downloading of physics datasets with offline support once cached. The simulation integrates a user-friendly GUI built on the YAPTIDE framework, enabling interactive setup, monitoring, and visualization without local installation or server dependence. Running simulations locally keeps sensitive patient data on the user's device, minimizing security risks. Immediate visual feedback and error tracking support fast simulation cycles for efficient research use. To demonstrate its robustness, the tool will be applied to replicate sophisticated hadrontherapy, brachytherapy, and FLASH radiotherapy simulations previously published and validated by the Geant4 collaboration.

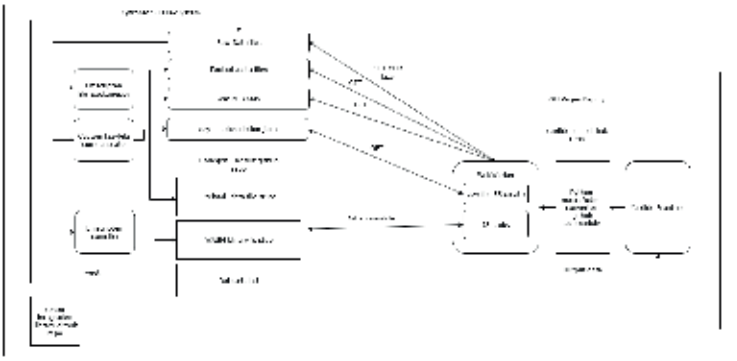

Fig.1. Toolkit for enhanced data sharing and collaboration

5. Conclusions and future work

This on-device, browser-based radiotherapy simulation framework merges the accessibility and ease of web applications with the security and privacy benefits of client-side computation. It addresses substantial practical and regulatory challenges by eliminating the need to upload sensitive health data for particle transport simulations.

Future research will focus on further optimizing performance using GPU acceleration APIs like WebGPU, expanding support for more complex simulation scenarios, and enhancing the user interface with real-time collaborative feature.

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Oral presentation

Extracting eye movement information from fMRI images

Cemal Koba, Jan K. Argasiński

Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland

{c.koba,j.argasinski}@sanoscience.org

Keywords: eye movements, fmri, fixation, resting state, stroke

1. Introduction

Functional magnetic resonance imaging (fMRI) is a widely used tool to study functional alterations after brain stroke. Along with neural activity, fMRI signal can be used to extract information about non-neural physiological activity such as respiratory and cardiac oscillations at low-level frequencies [1,2]. Eye movements can be also detected using fMRI signal from eye vitreous [3,4]. This information is valuable as it allows direct comparison between oculomotor activity and neural dynamics without the need of additional eye-tracker device.

2. Description of the problem

In fMRI images (T2* contrast), eye vitreous look bright and optic nerves are visible. However, those regions have low signal-to-noise ratio and the eyes look distorted. In addition, temporal resolution of eye movements are much faster that fMRI's temporal resolution, therefore it is harder to catch the eye position at each volum.

3. Related work

Previous work successfully detected eye position over time using fMRI images [5]. However, they have used a deep-learning-based model trained on healthy population and the output is one position for both eyes. There is a need for unsupervised model that can be applied in any kind of population and decides the position for both eyes separately in case the sample represents a special population.

4. Solution to the problem

We used an fMRI dataset of stroke patients healthy controls [5]. Data was scanned during a resting-state paradigm and subjects were asked to fixate on the center of the screen during the experiment. After applying conventional fMRI preprocessing steps [6] on the dataset, we applied an affine registration on eye regions. We aligned each fMRI volume of eye regions to the first time point and saved 6 motion parameters (translation and rotation in x, y, and z directions). The 6 parameters were used to create a composite measure called "frame-wise displacement", that shows the magnitude of movement compared to the first time point. This metric was used as a marker for eye movement information. The mean frame-wise displacement of each stroke patient (N = 84) was correlated with their lesion size (Spearman's r=-0.25, p=0.02) and NIHSS score (indicator of stroke severity, r=-0.28, p=0.01).

5. Conclusions and future work

Unsupervised linear methods are promising to derive eye movement information from fMRI images. The extracted information can be used investigate the relationship between neural

and oculomotor dynamics. The proposed method will be refined to characterize the exact location of the eyes in order to allow for more sensitive analyses.

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Oral presentation

New approaches to bioinformatics analysis in Leiden University Medical Center: bone marrow transplant in Thalasemia patients

Katarzyna Jurkowska[1,2], Gertjan Lugthart[2], Szymon M. Kiełbasa[2], Marek Kisiel- Dorohinicki[1]

[1]AGH University, al. A. Mickiewicza 30, 30-059 Krakow, Poland
[2]Leiden University Medical Center, Albinusdreef 2, 2333 ZG Leiden, Netherlands

kjurkowska@agh.edu.pl

Keywords: thalassemia, hematopoietic stem cell transplantation, single-cell RNA sequencing, graft rejection, bone marrow microenvironment

1. Introduction

Thalassemia is a genetic blood disorder characterized by impaired hemoglobin synthesis due to mutations affecting globin chain production. Management of the disease relies primarily on life-long blood transfusions and iron chelation therapy, procedures that considerably improve survival but are associated with severe complications, including iron overload, endocrine dysfunction, organ failure, and reduced quality of life. Allogeneic hematopoietic stem cell transplantation (HSCT) remains the only potentially curative option. However, despite significant progress, in thalassemia patients undergoing HSCT the rates of graft rejection and graft-versus--host disease (GvHD) are much higher than in other diseases requiring bone marrow transplantation. To improve outcomes, a deeper understanding of the molecular and cellular mechanisms governing donor–host interactions is required.

2. Description of the problem

The major challenge in HSCT for thalassemia is the hostile host bone marrow environment, which may prevent durable donor cell engraftment. In post-transplant samples, bone marrow shows a mixed cellular composition, with cells originating from both donor and recipient, and distinguishing their origin is technically demanding. Bulk assays cannot resolve this complexity, so specialized computational methods are required. Tools such as Vireo, which use natural genetic variation to assign cells to donor or host in single-cell RNA sequencing data, enable precise identification of cellular origin. Such integrative approaches, combining clinical insight with bioinformatics, are crucial for uncovering molecular determinants of graft success that go beyond standard HLA matching.

3. Related work

Previous studies have highlighted the impaired function of mesenchymal stromal cells in β-thalassemia, including reduced clonogenicity, defective differentiation, and altered secretion of key hematopoietic support factors. These abnormalities, often driven by iron overload and oxidative stress, compromise the bone marrow niche and may hinder donor stem cell engraftment. Although single-cell RNA sequencing has been successfully applied to characterize hematopoietic and immune heterogeneity in other contexts, its systematic use in thalassemia remains limited, and disease-specific microenvironmental mechanisms of transplant failure are still poorly understood.

4. Solution to the problem

We applied scRNA-seq to bone marrow samples obtained from healthy donors and thalassemia patients both before and after HSCT. Using e bioinformatics pipelines (Seurat, SingleCellExperiment) and visualization platforms (CellxGene), we were able to deconvolute the mixed cellular composition of post-transplant samples, accurately tracing the origin of cells and distinguishing donor- from recipient-derived populations. This approach enabled us to identify transcriptional differences between donor and patient cells, particularly at the late stages of erythropoiesis, where donor cells appeared to adopt stress-related or dysfunctional programs under the influence of residual thalassemic host cells and altered niche signals. Such interactions may play a central role in impaired engraftment and graft failure.

To strengthen these observations, additional strategies can be employed, including integration of scRNA-seq with genotyping data to improve donor–recipient cell assignment, the use of trajectory inference methods to capture dynamic lineage transitions, and cross-validation with proteomic or spatial transcriptomic data to map donor–host interactions within the bone marrow microenvironment.

5. Conclusions and future work

Our findings indicate that host–donor interactions within the thalassemic bone marrow niche can shape HSCT outcomes. Identified genetic and antigenic markers could be incorporated into extended donor–recipient matching protocols to reduce graft rejection rates.

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Oral presentation

Exploring EEG Features Structure for Neuroscreening: A Study of Dimensionality Reduction Techniques

Maja Marzec

Faculty of Physics UW, Ludwika Pasteura 5, 02-093 Warszawa

me.marzec3@student.uw.edu.pl

Keywords: : machine learning, dimensionality reduction, feature engineering, interpretability, XAI, PCA, ICA, UMAP

1. Introduction

Electroencephalography (EEG) is a cost-effective, non-invasive tool for monitoring brain activity, but the resulting signals are high-dimensional and noisy, making clinical interpretation challenging [1]. In computational medicine, particularly in neuroscreening as a rapid diagnostic aid, there is a need for automated models that reduce data complexity while preserving interpretability. This ensures healthcare professionals' trust in the results and optimizes both computational cost and processing time. Dimensionality reduction (DR) offers a promising solution by extracting compact latent representations from EEG-derived features without compromising clinical transparency.

2. Description of the problem

This study investigates how different dimensionality reduction (DR) techniques influence the classification of normal versus pathological EEGs. DR was applied to hand-crafted features - covariance matrices, power spectral densities (PSD), and coherence measures, computed at both the local (6-second frame-level) and global (recording-level, median-aggregated by frames) scales. This dual representation captures overall signal trends as well as short-term variations. Each feature vector consists of 2850 elements per frame/ recording, which means that training effective models on such high-dimensional data typically requires a large number of training samples [2]. Properly applied dimensionality reduction can make it feasible to train models on smaller EEG datasets, which is particularly valuable in biomedical applications where data are scarce and difficult to obtain. The main challenge is to achieve computational efficiency and interpretability while preserving diagnostic accuracy comparable to that obtained with the full original feature set.

3. Related work

The dataset, Gradient-Boosted Ensemble (GBE) model, and original features are sourced from [2]. Principal Component Analysis (PCA) is commonly used for dimensionality reduction, while Independent Component Analysis (ICA) is primarily applied in EEG analysis for artifact removal [3]. Uniform Manifold Approximation and Projection (UMAP) is used for visualizing high-dimensional data because it preserves the topological structure when projecting into lower dimensions, such as 2D or 3D. Investigating ICA and UMAP for dimensionality reduction of input features in classification models represents an innovative approach that has not been previously explored.

4. Solution to the problem

IThe implemented framework combines systematic component selection, classification, and

interpretability. First, a variance-based Meaningful Components Selection criterion was applied, retaining components until 95% of cumulative explained variance was captured. This ensured DR without neglecting diagnostically relevant information. Next, to enhance clinical transparency, an innovative Selective Activation algorithm was developed. The Selective Activation algorithm back-projects variance-preserving components onto original EEG feature spaces, enabling temporal and spectral mapping that supports physiological interpretation [5]. Finally, classification performance was evaluated using a Gradient-Boosted Ensemble (GBE) model trained on (i) original scaled features, (ii) PCA-reduced features, and (iii) ICA-reduced feature.

Fig. 1. Workflow chart summarizing the EEG Feature Extraction + DR + Interpretability + ML pipeline.

5. Conclusions and future work

With variance-based component selection, dimensionality reduction preserved GBE classification performance while improving interpretability and generalizability, supporting robust EEG assessment across heterogeneous clinical contexts. These findings confirm that reduced feature spaces can provide both computational efficiency and clinical transparency, making them well suited for neuroscreening applications.

Future work will extend the Selective Activation algorithm into dedicated software to facilitate integration into clinical workflows and to strengthen healthcare professionals' trust in automated assessment tools. In parallel, exploring unsupervised and neural-network-based models may uncover structure beyond hand-crafted features [6], further enhancing generalizability across heterogeneous datasets and improving applicability in real-world computational medicine.

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Towards the Development of Non-Invasive Electrical Impedance Spectroscopy-based Oral Cancer Diagnosis System

Malwina Matella[1,4], Rachel Furmidge[2,4], Zhicheng Lin[3,4], Helen Colley[2,4], Craig Murdoch[2,4], Zi-Qiang Lang[3,4], Dawn Walker[1,4]

[1] School of Computer Science, University of Sheffield, UK
[2] School of Clinical Dentistry, University of Sheffield, UK
[3] School of Electrical and Electronic Engineering, University of Sheffield, UK
[4] Insigneo Institute for In Silico Medicine, University of Sheffield, UK

{m.matella, d.c.walker}@sheffield.ac.uk

Keywords: Oral Cancer Diagnosis, Electrical Impedance Spectroscopy, Tissue Engineering, Finite Element Modelling, Machine Learning

1. Introduction

Head and neck cancer remains the seventh most common type of cancer worldwide, with oral squamous cell carcinoma (OSCC) being one of its most prevalent subtypes [1]. In 2020, more than 377,000 new cases of OSCC were reported, resulting in nearly 178,000 deaths [1]. Despite advances in treatment, the overall 5-year survival rate remains low at 54%, largely due to latestage diagnosis [2]. In contrast, early detection can improve survival rates – up to 90% [2].

2. Description of the problem

The current golden standard in the diagnosis of OSCC is a scalpel biopsy, which is a painful procedure with long turn-around times. Additionally, in the case of mild to moderate dysplasia, the biopsy often needs to be repeated. The low 5-year survival rate associated with the late diagnosis indicates that there is a continuing need for an earlier oral cancer detection or oral cavity screening programme amongst patients of increased risk. One potential solution is a diagnostic tool based upon electrical impedance spectroscopy (EIS), a technology permitting non-invasive and real-time identification of cancerous changes in various biological tissues based on the influence of cellular level tissue structure on the opposition to the flow of an alternating electrical current.

3. Related work

The use of EIS in cancer diagnosis has been investigated from the late 1990s, resulting in the cervical cancer diagnosis commercial device, ZedScan, that demonstrates Area Over the Curve (AUC) of 0.887 for early cervical cancer detection when paired with colposcopy [3]. Our current work relating to the use of EIS in the more complex scenario of early oral cancer detection builds upon a small pilot study exploring the potential for EIS to distinguish cancerous and potentially malignant lesions from healthy oral epithelium in vivo [4]. Despite promising results (significant differences in the EIS of cancer and high-risk lesions versus low-risk lesions and controls), a deeper understanding on the impact of tissue composition and structure in health and pathology on their electrical behaviour is needed before the deployment of EIS in the clinic.

4. Solution to the problem

In the current study, we explore the feasibility of EIS measurement to enhance the diagnosis of oral cancer by integrating tissue engineering (TE), finite element (FE) and machine learning

(ML) models to develop a prototype oral cancer detection system. Due to the lack of the necessary certification for the in vivo use of our current EIS instrumentation, TE oral epithelium constructs are cultivated using healthy and cancerous cell lines. EIS measurements are performed on the mature TE samples, which are subsequently prepared for histology. Histology images provide morphological information which are the basis of Virtual Oral Tissues i.e. tissuespecific multiscale FE models. The latter are deployed to investigate the impact of tissue characteristics (morphology and composition) on different EIS spectra features, and to augment the TE-derived EIS dataset for classification study. Four ML models were trained on the simulated spectra and tested on the TE EIS data. Initial results (Fig. 1) show promising agreement between the EIS spectra obtained from TE models and FE simulations, and subsequent classification study results exhibit the best separability using a decision tree model with AUC=0.913 after 100-fold cross validation.

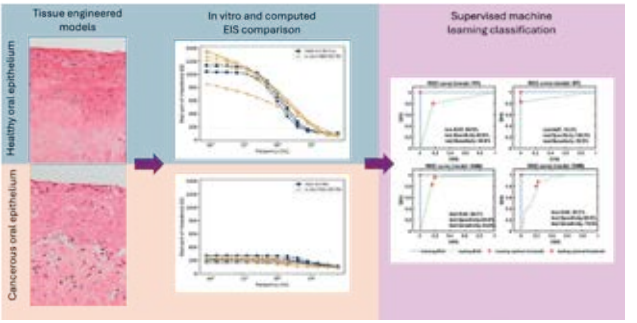

Fig. 1. Preliminary results showing (from left to right): the TE healthy and cancerous oral epithelium, comparison between the in vitro measured (yellow) and simulated (navy blue) EIS spectra, and ROC curves resulting from a classification task using different supervised ML models.

5. Conclusions and future work

In this preliminary study, we developed a process combining tissue engineered and computational models to classify healthy and cancerous oral epithelium using electrical impedance spectroscopy. Preliminary data confirmed the utility of the FE modelling and ML in predicting and classifying the EIS spectra of healthy and cancerous oral epithelium constructs. This provides proof-of-concept that ML models informed by simulation-augmented EIS data could ultimately form the basis of a clinical diagnosis method for oral cancer diagnosis. In the future work we plan to adapt the existing framework to explore different stages of dysplasia, to calibrate and validate the FE model given the parameters from histopathology and transmission electron microscopy (TEM) images. Following the required certification for medical devices, the definitive aim will be to carry out a follow-up in vivo study, where additional patient history could enhance the ML classifiers accuracy and interpretability.

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Oral presentation

Portable Auscultation Device for Perfusion Evaluation - 5PAudio, a novel personalized Monitoring and Prediction approach

Michael Friebe, Katarzyna Heryan, Hamza Oran, Dominik Rzepka

AGH University of Krakow, Faculty of Computer Science, Healthtech Innovation Group, 30-059 Kraków, Poland

{friebe, heryan, oran, rzepka}@agh.edu.pl

Keywords: Acoustic Sensing, Perfusion Monitoring, Stroke Prediction, Acoustic Body Atlas

1. Introduction

Stroke imposes substantial health and economic burdens worldwide, yet timely identification of high-risk individuals remains challenging. Imaging-based screening, such as Doppler ultrasound, is resource intensive and unsuitable for frequent or widespread use [1–3]. Recent advances in biomedical acoustics show that vascular sound patterns can reveal early disease indicators. 5PAudio—a handheld device generating an individualized vascular audio biomarker (Fig. 1). Its portability and affordability make it suitable for routine and home-based monitoring, addressing a critical gap in preventive healthcare.

2. Description of the problem

Carotid artery stenosis is a major cause of ischemic stroke, often progressing silently. Current diagnostic imaging requires specialized equipment and expertise, limiting accessibility. Post-stenting restenosis monitoring shares these limitations. An accessible, repeatable tool for early detection and follow-up could enable timely interventions, particularly in underserved populations.

3. Related work

Vascular auscultation has been examined for disease detection, with studies showing that carotid blood flow sounds are stable and unique. Phonocardiography for heart disorders and respiratory audio analysis for lung disease demonstrate the broader diagnostic value of biomedical sound analysis. Yet, no established portable system exists for vascular audio biomarker-based stroke prevention [3,4].

4. Solution to the problem

5PAudio uses a handheld vibroacoustic sensor (see Figure 1) to capture carotid blood flow sounds. Advanced algorithms segment the signal and extract features indicating turbulent or restricted flow. The resulting personalized biomarker can be applied to:

1. Early screening for asymptomatic stenosis,
2. Progression tracking in diagnosed cases,
3. Restenosis detection after stenting.

Our Audio4Prevention extension aims to combine vascular, respiratory, and joint sound biomarkers for multi-organ health monitoring in the future [4-6].

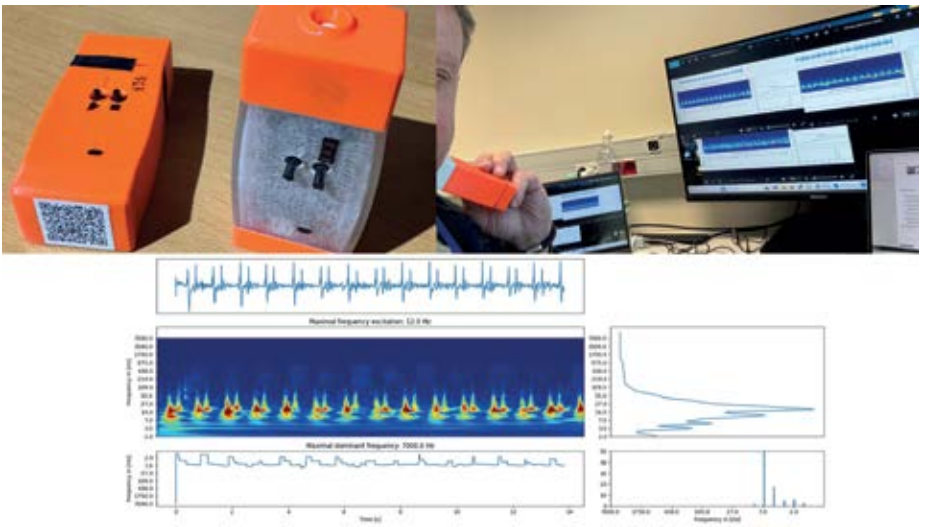

Fig. 1. The prototype devices on the top left. The acquisition screen shows the frequency spectrum of the individual. Every individual has a unique frequency profile that can be used as an audio biomarker as part of a digital health twin.

5. Conclusions and future work

A vascular audio biomarker device offers a scalable, non-invasive means of preventing stroke and supporting long-term health monitoring. Future goals include refining analysis algorithms, expanding biomarker libraries, and validating effectiveness through large-scale clinical trials, with integration into telemedicine systems for broad access [7-9].

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Oral presentation

Preliminary Evaluation of Virtual Reality Simulator for Surgery Training in International Medical Students

M. Wójcikowski[1], D. Dall'Alba[2], S. Martyniaki[1], R. Szydlak3, P. Walecki[3], A. A. Kononowicz[3], P. Korzeniowski[1]

[1]Sano Centre for Computational Medicine
[2]Department of Engineering for Innovation Medicine, University of Verona, Italy
[3]Department of Bioinformatics and Telemedicine, Jagiellonian University Medical College

p.korzeniowski@sanoscience.org

Keywords: Surgical Simulation, Medical Education, Cholecystectomy

1. Introduction

Virtual Reality (VR) simulators are promising instruments for enhancing medical education [1], particularly in the field of Robotic Assisted Surgery (RAS), where the high cost of training equipment is a significant barrier. In contrast to laparoscopic training, which can be done with inexpensive trainer boxes [2], RAS practice requires access to costly robot simulators. This study examines the experiences and perceptions of 67 international medical students with a VR headset-based robotic surgery simulator, focusing on evaluating its usability and educational worth.

2. Description of the problem

The simulation of complex, non-linear soft tissue behavior poses a major computational challenge, especially on low-power, standalone VR hardware. A critical requirement for a useful surgical simulator is a robust physics engine that performs in real-time. This means achieving a high physics refresh rate (1 kHz) for simulation accuracy and stability, while also maintaining a high graphics rendering rate (90 Hz) to deliver a smooth, immersive experience and reduce the risk of VR-induced motion sickness.

3. Related work

To address the challenge of simulating non-linear tissue behavior, this project utilizes the Extended Position-Based Dynamics (XPBD) method [3]. The advantage of XPBD lies in the local nature of its non-linear Gauss-Seidel process, which helps to avoid many of the difficulties found in global, matrix-based solvers. This allows it to stably manage both equality constraints (like deformations) and inequality constraints (like collisions). Recent research has confirmed that XPBD is a competitive option when compared to more advanced methods in terms of its accuracy, stability, performance, and ease of implementation [4-6].

4. Solution to the problem

The developed simulator functions as a native standalone application on Meta Quest 2, 3/3S, and Pro headsets. This setup achieves a real-time soft tissue simulation with a 1 kHz refresh rate and a 90 Hz graphics rendering rate. The chosen procedure is the cholecystectomy. As illustrated in (Fig. 1), the simulation covers the dissection of the hepatocystic triangle, the clipping and cutting of the cystic duct and artery, and the separation of the gallbladder from the liver. This study used a quantitative survey distributed to 67 international medical students; 58% of the participants were

female, and 71% had prior experience with VR headsets. The majority of participants reported a positive user experience, and most did not encounter simulator sickness or eye discomfort. A majority (over 80%) of respondents believed the simulator improved their understanding of anatomical structures and surgical procedures. More than 75% regarded the simulator as a valuable educational tool and would recommend it to their peers.

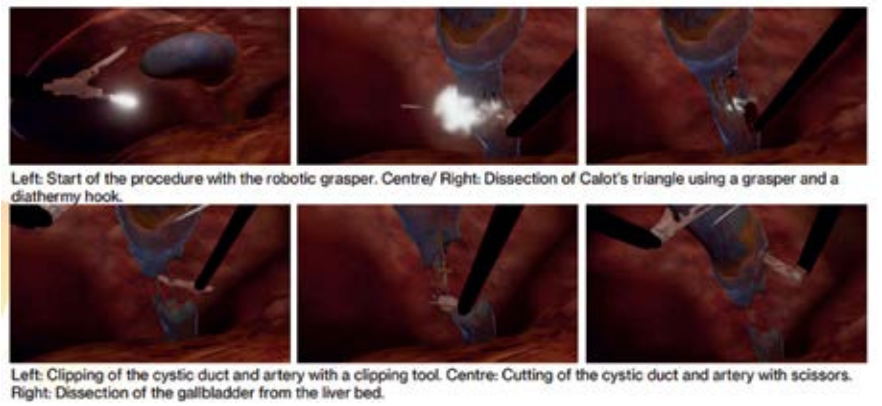

Fig. 1. Steps of cholecystectomy procedure.

5. Conclusions and future work

Open-ended responses from the survey provided valuable feedback. Students appreciated the opportunity to practice procedures without risk to patient safety, the immersive quality of the VR environment, and the ability to engage in repeated practice. Common suggestions for improvement included enhancing the realism of the simulation, especially regarding tissue interaction, and expanding the variety of available procedures to include complex scenarios and anatomical variations. Additional feedback emphasized the need for more intuitive user interfaces that are optimized for VR devices. VR surgical simulators demonstrate significant promise for transforming medical education.

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Oral presentation

Decoder Conditioning with Tabular Data for Enhanced 3D Image Segmentation

Tomasz Szczepański[1], Michal K. Grzeszczyk[1], Szymon Płotka[1], Arleta Adamowicz[2], Piotr Fudalej[2], Przemysław Korzeniowski[1], Tomasz Trzciński[3], Arkadiusz Sitek[4]

[1]Sano Centre for Computational Medicine, Kraków, Poland
[2]Jagiellonian University Medical College, Kraków, Poland
[3]Warsaw University of Technology, Warszawa, Poland
[4]Massachusetts General Hospital, Harvard Medical School, Boston, MA, USA

t.szczepanski@sanoscience.org

Keywords: Conditioning, Tabular data, Non-Imaging, Segmentation

1. Introduction

When studying the expression of genes at the RNA level, the key problem becomes mappin- Recent advancements in deep learning have achieved strong performance in 3D medical image segmentation across various domains. However, these models typically rely on large, expertly annotated datasets, which are expensive to produce, and often fail to generalize across clinical centers and diverse patient populations.

2. Description of the problem

While some studies have explored architectural refinements or loss-based improvements, the integration of structured tabular data, such as clinical metadata or label-derived properties, remains underutilized in segmentation. Such data can encode valuable contextual information but is often missing, inconsistent, anonymized, or lacking a direct semantic correspondence to pixel-level labels. Existing approaches for incorporating tabular data are more common in regression tasks, where strong, explicit correlations between covariates and outcomes exist, such as predicting disease progression or birth weight. In segmentation, where labels are high-dimensional and relationships with metadata are indirect, the challenge of effective integration is greater.

3. Related work

Methods such as DAFT [1] and TabAttention [2] have shown benefits in regression tasks by exploiting the clear linkage between tabular variables and target measures. In segmentation, some progress has been made, for example, with INSIDE [3], which incorporates limited non-imaging metadata like cardiac phase or anatomical slice position into 2D networks. However, these approaches rely on predefined categorical metadata and operate in constrained settings. Importantly, few works have explored decoder-level conditioning in 3D segmentation networks, and none have proposed a framework that leverages label-derived embeddings during training without requiring such data at inference.

4. Solution of the problem

We introduce DeCode, a decoder conditioning framework for 3D medical image segmentation that learns to embed shape-derived features from ground-truth labels during training. Radiomics-based shape metrics, such as surface area, compactness, and elongation, are computed using the PyRadiomics library and embedded into a conditioning vector. This vector modulates the decoder through affine transformations applied to internal feature maps, with transformation

parameters generated by a hyper-network. Unlike batch normalization, this conditioning operates at the individual sample level, enabling fine-grained control of feature activations. During inference, when labels are unavailable, DeCode predicts the conditioning embedding directly from the encoder's latent representation, allowing the network to benefit from label-informed structure without manual annotations. We implement DeCode in a U-Net-style architecture with four encoder and four decoder blocks, inserting conditioning layers after skip connections. In addition to the primary segmentation loss, two auxiliary objectives are used: (1) minimizing the distance between predicted and true embeddings, and (2) regressing predicted radiomics features to their actual values. We evaluate DeCode on two tasks: a synthetic dataset, 3DeCode, inspired by CLEVR-Seg but extended to 3D, and a clinical dataset of cone-beam CT (CBCT) scans of teeth. On synthetic shape-based segmentation tasks, DeCode outperforms unconditioned baselines, achieving over 94% Dice score on challenging mixed-shape-and-size scenarios compared to near-random baseline performance. On CBCT scans, DeCode achieves superior accuracy on external datasets from different centers, approaching the performance of an upper bound that uses ground-truth conditioning features at inference. Ablations confirm that both the conditioning mechanism and auxiliary regression loss significantly contribute to performance, while random embeddings at inference degrade results. The method also requires fewer parameters and less training time than heavier alternatives such as VNet.

5. Conclusions and future work

DeCode demonstrates that decoder conditioning with label-derived embeddings can improve 3D segmentation accuracy and generalization without requiring inference-time metadata. This approach expands the toolkit for data-efficient segmentation, making it suitable for scenarios with limited computational resources. Limitations include reliance on predefined radiomics features, which do not capture spatial relationships or object context, and potential training instability on small datasets. Future research could explore end-to-end learning of embeddings directly from masks, integration of richer spatial and relational information, and extensions to multi-organ or temporal segmentation.

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Oral presentation

Advancing quality assurance of ion beam radiotherapy for cancers

Mateusz Wójcik[1,3], Leszek Grzanka[1,2], Jeppe Brage Christensen[3]

[1]AGH University of Krakow, al. Mickiewicza 30, 30-059 Kraków, Poland
[2]IFJ PAN, Radzikowskiego 152, 31-342 Kraków, Poland
[3]Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen, Switzerland

mwojci@student.agh.edu.pl, leszek.grzanka@ifj.edu.pl, jeppe.christensen@psi.ch

Keywords: HPC, medical simulation, ion chamber, particle therapy, recombination

1. Introduction

Radiotherapy has been a key component in cancer treatment for more than 100 years. Beyond conventional radiotherapy with photons, therapy with ions, known as particle therapy [3], is increasing worldwide. Furthermore, the emerging concept of ultra-high dose rate (UHDR) radiotherapy, or FLASH, offers the potential for an even greater reduction in radiation-induced toxicities. Prior to all therapies with particles, a thorough quality assurance is conducted with ionisation chambers. Measurements that rely on multiple corrections, including so-called ion recombination.

2. Description of the problem

Ionization chambers are considered the gold standard for determining dose in clinical and experimental settings, as they measure ionizing radiation by collecting charges produced in the medium [6]. A major challenge arises because some ions recombine before collection, thereby reducing the measured charge. The recombination correction factor must therefore be accurately determined to ensure a correct treatment of the patient.

Analytical theories describing this effect were developed in the 20th century, primarily by Jaffé [2] and later extended by Boag. While these models work well at low dose rates—where the recombination factor is below 1 %—at higher dose rates the factor may drop by up to 50%. In such cases, analytical theory fails to provide accurate corrections. To tackle this long-standing challenge and enable precise determination of ion recombination correction factors, we introduce the first dedicated numerical toolkit that leverages modern, state-of-the-art computational methods to faithfully solve the underlying physics.

3. Related work

Research in this direction has been motivated by the FLASH initiative, as UHDR radiotherapy moves toward clinical translation. Our toolkit IonTracks is a direct continuation of prior work [1], but introduces a fundamentally different simulation strategy, allowing more detailed modeling of recombination and transport phenomena. Other studies rely on techniques that cannot account for the high ionisation density within particle therapy tracks.

4. Solution to the problem

The implementation leverages the open-source FEniCS project [5], enabling efficient numerical solutions of partial differential equations (PDEs) relevant to charge transport and recombination. Python-based front-end code provides ease of use, while C++ back-end libraries deliver high computational performance. A dedicated abstraction layer allows users to flexibly modify

simulation parameters without editing source code. Considerable effort was devoted to ensuring numerical stability and minimizing computational errors. Various meshing strategies were tested using gmsh [4], from uniform to adaptive approaches, and results were visualized with ParaView. The software is designed to efficiently utilize multi-threaded execution, enabling both seamless use on personal computers and scalable performance on HPC machines such as Ares.

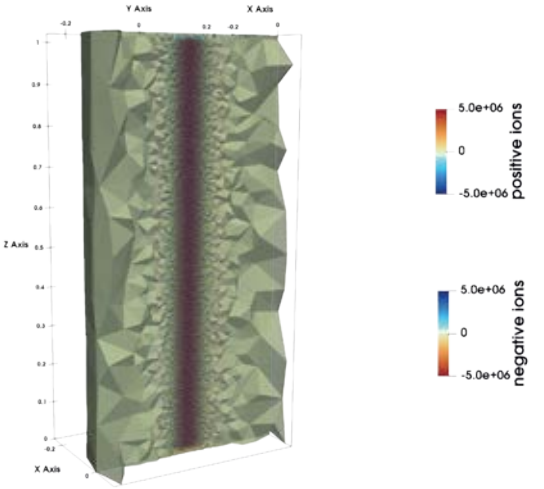

Fig. 1. Example simulation of a parallel plate ionisation chamber (yellow) where the charge carriers (red and blue) from an ion track have been simulated.

5. Conclusions and future work

This computational framework strengthens the accuracy of ionization chamber measurements for quality assurance in heavy ion beam applications, thereby supporting the increasing global implementation of ion beam therapy in cancer treatment.

The next step will be to extend the simulation framework to support so-called MR-guided linacs, which still remains an unsolved problem, as the magnetic field impacts the movements of the charged carriers.

Acknowledgements. We acknowledge the support of EU: Traceable dosimetry for FLASH radiotherapy:// flash-dose.eu/, as well as ACK Cyfronet AGH for providing computer facilities and support within computational grant no. PLG/2025/018530.

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Oral presentation

Digital Twin-Based Prognostic Modeling in Aortic Coarctation and Hypoplastic Aortic Arch

Krystian Jędrzejczak[1], Rawan Abuzinadah[2], Paola Franceschi[3,4], Julio Sotelo[5], Malenka M. Bissell[2], Łukasz Makowski[1]

[1]Warsaw University of Technology, Faculty of Chemical and Process Engineering, Waryńskiego 1, Warsaw, Poland
[2]University of Leeds, Leeds Institute of Cardiovascular and Metabolic Medicine, Leeds, UK
[3]Pediatric and Adult CardioThoracic and Vascular, Oncohematologic and Emergency Radiology Unit, IRCCS University Hospital of Bologna, Via Massarenti 9, 40138, Bologna, BO, Italy
[4]Department of Surgical and Medical Sciences (DIMEC), University of Bologna, Bologna, Italy
[5]Departamento de Informática, Universidad Técnica Federico Santa María, Santiago, Chile

krystian.jedrzejczak@pw.edu.pl

Keywords: CFD, congenital heart defects, personalized medicine, digital twin, ResNet

1. Introduction

Congenital heart defects are identified in around 1% of newborns [1]. In particular, defects such as aortic coarctation and hypoplastic aortic arch can cause symptoms in neonates such as poor feeding tolerance, respiratory distress, cold extremities, diminished or absent femoral pulses, pallor, and tachycardia.

2. Description of the problem

Current procedures for identifying congenital cardiovascular defects rely primarily on fetal echocardiography (ECHO) during pregnancy [2]. However, the limited resolution of this imaging technique, combined with the growing prevalence of maternal obesity, makes it particularly challenging to diagnose conditions such as aortic coarctation and hypoplastic aortic arch. As an alternative, other imaging methods such as magnetic resonance imaging (MRI) may be considered, although MRI is not yet a standard procedure during pregnancy or in newborns [3], [4]. Moreover, in the case of small vessels, MRI may not provide sufficient image quality. Therefore, it is necessary to use artificial intelligence techniques to upscale and enhance the quality of medical images.

3. Related work

The use of magnetic resonance imaging combined with artificial intelligence for the development of new diagnostic methods is an active area of research at the intersection of medicine and engineering [3], [4], [5]. This topic strongly resonates within the scientific literature, reflecting growing interest in interdisciplinary approaches to improving diagnostic accuracy and patient outcomes.

4. Solution to the problem

As part of the study, 4D Flow MRI examinations were conducted on newborns after obtaining approvals from the bioethics committee and informed consent from the children's legal guardians. The acquired 4D Flow MRI data were subsequently upscaled using a neural network to improve spatial resolution and enhance the signal-to-noise ratio [5], [6]. These data were used

to develop both a generalized numerical model of aortic coarctation and personalized models, which served to identify key parameters enabling the diagnosis of these congenital cardiovascular defects. The results of the CFD analyses were compared with data obtained from the 4D Flow MRI using the 4D Flow MRI Toolbox for MATLAB [7] and the Cass software.

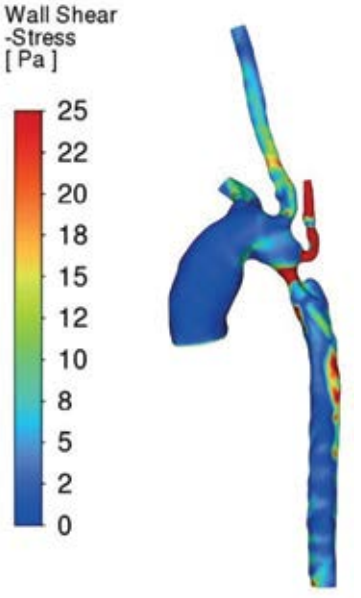

Fig. 1. Wall shear stress [Pa] distribution contours for an newborn with aortic coarctation.

5. Conclusions and future work

Our research enabled the identification of key parameters essential for the accurate diagnosis of aortic coarctation and hypoplastic aortic arch in infants, based on 4D Flow MRI data enhanced by artificial neural networks and supported by CFD simulations.

Acknowledgements. Research was funded by Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme.

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Oral presentation

Towards personalised dynamic models of the cardiovascular system

Karolina Tlałka[1,2], Ian Halliday[2], Andrew Narracott[2], Maciej Malawski[1,3]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Division of Clinical Medicine, The University of Sheffield, Western Bank, S10 2TN, Sheffield, UK
[3]Faculty of Computer Science, AGH University, Al. Mickiewicza 30, 30-059, Kraków Poland

{k.tlalka,m.malawski}@sanoscience.org, {i.halliday, a.j.narracott}@sheffield.ac.uk

Keywords: medical simulations, personalized medicine, Virtual Human Twin, heart-brain interactions, cardiovascular modelling, personalisation, sensitivity analysis

1. Introduction

Personalisable physics-driven modelling is a powerful tool to support clinical decisions and medical research [1]. There are some basic requirements, which must be met by models to promote clinical utility: (i) ability to represent physiological processes, (ii) simplicity, which decreases computational costs of model quantification and personalization, (iii) explainability, which is crucial to foster clinical trust in the model. In this work, we present our approach to personalization of reduced-order cardiovascular (CV) models with neuro-regulation.

2. Description of the problem

Currently, most CV models are assumed to have constant input parameter values. However, homeostasis is constantly challenged by external factors, such as orthostatic stress [2]. In a healthy subject, regulation mechanisms, such as baroreflex (neural control of the CV system), constantly modify the physiological state in response to those changes [3]. In patients with baroreflex impairment, symptoms such as dizziness and fainting can occur during their exposure to the orthostatic stress [4]. Incorporating “active” baroreflex control into a “passive” CV system model allows one to analyse conditions connected with baroreflex failure [2]. This leads to a more accurate model, but also increases the computation time, and introduces new parameters which are notoriously difficult to measure, what makes personalization harder [2].

3. Background

The zero-dimensional approach is widely used for modelling the entire CV system [5-7]. Baroreflex models are inspired by physiological mechanism of modifying the properties of CV system by neural control [3,5,7]. They are described within control theory, providing regulation of arterial pressureby negative a feedback mechanism. The control problem is usually analysed at a local scale [3], which is a computationally efficient solution, but it may not be accurate, because of the nonlinearity of the model, introduced by e.g. cardiac function [1,2]. Computational expense arising from the need for a global analysis and the number of parameters forces one to focus on model reduction i.e. parsimony of CV models, parameter subset selections and model quantification [2] as an essential prelude to any attempt at personalization.

4. Solution to the problem

In this research we are focused on the whole process of model development. We gradu-

ally increase the structural complexity of the CV model, to find the solution which is physiologically adequate and easy to personalize. We quantify the global sensitivity (see [1]) and orthogonality of candidates, to improve understanding of physiological processes connected with orthostatic response and analyze interactions between parameters and identify the most influential [2]. We use this knowledge to inform personalization process and achieve patient-specific models of human response to orthostatic challenge [2]. We have developed two CV models of graded complexity and performed local and global sensitivity analysis, to determine which input parameters influence pressures in the system and cardiac output [1] in the absence of any disturbance. We observed significant differences between global and local sensitivity patterns, for a model with a systemic and pulmonary circulation [1], which suggests the importance of higher order interactions between parameters and a need for global methods in characterizing the problem. Currently we are working on the personalization of CV models with a four-chamber heart, in the response to induced central hypovolemia [2]. We utilize global sensitivity analysis and optimization to fit our model response to the experimental data [2] such as [8]. Throughout, we use the Julia programming language, leveraging its extensive libraries, which allow one efficiently to solve our differential equation problem formulation and the associated global optimization problems. We utilize High Performance Computing, to perform parallelized global sensitivity analyses, screening of the search space, and optimization [2].

5. Conclusions and future work

Personalisation of dynamic CV models is a very challenging task, because of high uncertainty in input parameters, nonlinearity and computational expense. In this research, we address the balance between simplicity and physiological relevance. We will seek for a principled, versatile and portable (ideally universal) method for calibration of CV models to different orthostatic challenges. This will allow us quickly to conduct in silico studies of various experimental settings and move our models one step closer to the clinic.

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Oral presentation

Comparison of MRI-derived Cardiac Power with and without Deep Learning Acceleration

Grace Faulkner[1,2], Paul Morris[1,2,3], Ian Halliday[1,2]

[1]Division of Clinical Medicine, School of Medicine and Population Health, University of Sheffield, Sheffield S10 2TN, UK
[2]INSIGNEO Institute for in silico Medicine, Sheffield S1 3JD, UK
[3]Department of Cardiology, Sheffield Teaching Hospitals NHS Foundation Trust, Sheffield S10 2JF, UK

gfaulkner1@sheffield.ac.uk

Keywords: MRI, deep learning, cardiac power, cardiovascular

1. Introduction

Cardiac power at rest and in exercise can provide useful diagnostic information across a range of cardiovascular pathologies. Historically, this informative metric could only be quantified invasively, limiting its clinical use. However, a recent method derives cardiac power non-invasively using volumes derived from cardiac MRI (CMR) [1]. This method has been tested and validated at rest [2], but further work is needed to develop this method for use during exercise.

2. Description of the problem

Data acquisition during exercise is complex; motion within the MRI scanner can cause artefact in the acquisitions, leading to low-quality or unusable results. Exercise within the bore of the scanner is possible using a compatible supine cycle ergometer, but testing by this group has revealed the acquisition is still affected by artefact. Furthermore, it has been shown in the literature that acquisition longer than four seconds after the cessation of exercise causes significantly different end-systolic and end-diastolic volumes (ESV and EDV, respectively) [3]. To overcome this, the acquisition process can be accelerated using deep learning software which under-samples the k-space to reduce the scan time. The uncertainty in the volumes and cardiac power calculated using this accelerated method remains to be quantified. In this work we will compare the cardiac power at rest for one participant as a case study, both with and without a commercial deep learning algorithm to quantify the inherent uncertainty of the deep learning acceleration of left-ventricular power.

3. Related work

The foundation for the non-invasive cardiac power quantification is by Seemann et al. who use a 0D elastance model to relate the volume to the pressure in the chamber [1]. This method was optimised by previous work in this group to validate the choice of elastance model used [4].

4. Solution to the problem

A single participant (28 year old male) was used as a test case. CMR was performed on a 1.5-Tesla Siemens Signa Artist system (Siemens Healthineers AG, Erlangen, Germany) and analysed using Research software, MASS, (Geest, Leiden). Brachial systolic and diastolic pressure were also collected using a sphygmomanometer. Short-axis stacks were taken at rest, once with the deep learning acceleration, sonic DL (Siemens Healthineers AG, Erlangen, Germany), and once without. All other parameters were unchanged. The corresponding pressure was recovered using a

double cosine elastance as previously described [4]. The cardiac power was derived from the area of a plot of the pressure-volume loop. See Fig 1.

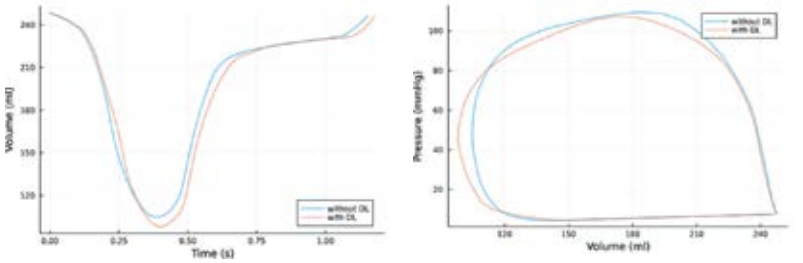

Fig. 1. (*Left*) time-series volume (*Right*) pressure-volume loops for the case study participant. Blue traces denote data derived without sonic DL, red denote the results when deep learning acceleration was used.

HR and cuff pressure were similar during both acquisitions, indicating the participant was in the same physiological state. The difference between HRs in both acquisitions was 1.1 bpm (2.1%) and the difference in the estimated end-systolic pressure was 2.1 mmHg (1.9%) for this participant.

Volumes were also closely aligned between the two methods. The difference in ESV was greater than the difference in end-diastolic volume but still within acceptable limits (ESV, 6.8 ml (6.5%); EDV, 0.2 ml (0.1%)). The resulting cardiac power was therefore similar between the two volume acquisitions, with a difference of 0.01J (0.64%).

5. Conclusions and future work

This case study suggests that using deep learning acceleration has little impact on the accuracy of the acquisition. These results are limited, as they were tested for one healthy volunteer at rest, but are promising for future testing of patients and in the exercise state, where the length of acquisition would be obstructive without deep learning acceleration.

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Oral presentation

Active Learning Virtual Screening of Ultra-Large Chemical Libraries: Scalable Docking with Uncertainty Quantification

Adam Sułek[1], Jakub Klimczak[1], Tomasz Danel[1,2], Jakub Jończyk[1,3], Tomasz Kosciolek[1], Barbara Pucelik[4]

[1]Sano Centre for Computational Medicine, Czarnowiejska 36, 30-054 Kraków, Poland
[2]Faculty of Chemistry, Jagiellonian University, 30-387 Kraków, Poland
[3]Faculty of Pharmacy, Jagiellonian University Medical College, 30-688 Kraków, Poland
[4]Łukasiewicz Research Network, Kraków Institute of Technology, 30-418 Kraków, Poland

{a.sulek,j.klimczak,t.danel,j.jonczyk,t.kosciolek}@sanoscience.org,
barbara.pucelik@kit.lukasiewicz.gov.pl

Keywords: HPC, Active Learning, Virtual Screening, Molecular Docking, Drug Discovery

1. Introduction

As an illustrative case, we focus on LasR, a key virulence regulator and biofilm inducer in P. aeruginosa. For this target, only sparse experimental activity labels are available, rendering data-driven supervised modeling infeasible. Consequently, structure-based methods such as molecular docking remain the primary strategy. Navigating ultra-large chemical libraries such as the 1.7 B compound SAVI collection, however, poses a major computational challenge for structure-based drug discovery. Traditional brute-force docking of such a library would require on the order of ~270,000 CPU hours for 1 B ligands (assuming ~1 second per docking on a single CPU). In contrast, our active learning (AL) workflow completes a single iteration in ~12 h on high-performance computing (HPC) infrastructure, while retaining scaffold diversity and hit quality. This highlights the need for scalable, uncertainty-aware machine learning approaches to make billion-scale screening feasible.

2. Description of the problem

Current approaches to large-scale docking either rely on heuristic filtering or exhaustive enumeration, both of which risk losing promising scaffolds or incurring prohibitive computational costs. While docking a 1B-compound library can be feasible within ~2 months on well-provisioned HPC infrastructure, scaling to ultra-large collections such as the 69B-compound SAVI expansion becomes practically impossible. Moreover, drug discovery campaigns rarely focus on a single molecular target—in practice, the entire screening process often needs to be repeated across multiple proteins or pathways, further multiplying the computational demand.

3. Related work

Recent advances have demonstrated the viability of billion-scale docking campaigns: Liu et al. screened 1.7 billion SAVI/ZINC22 molecules against AmpC β-lactamase, requiring ~2.1 million CPU-hours (~1 month on 3,000 cores), and experimentally validated over 1,500 compounds, confirming that larger libraries improve hit rates and scaffold diversity [1]. In contrast, machine learning with AL has been shown to reduce the docking workload by ~90%, achieving comparable enrichment while only sampling ~10% of the library, thus providing an effective ~10-fold acceleration of virtual screening [2].

4. Solution to the problem

We initiated the workflow by docking 100,000 structurally diverse SAVI compounds with SMINA on HPC resources. A supervised regression model was then trained on the resulting docking scores using extended-connectivity fingerprints. To incorporate AL, we employed Monte Carlo dropout, estimating predictive uncertainty from multiple stochastic forward passes and guiding selection with an acquisition function. Compounds were prioritized for subsequent docking based on both predicted binding affinity and model uncertainty, and the model was iteratively refined with each newly docked batch.

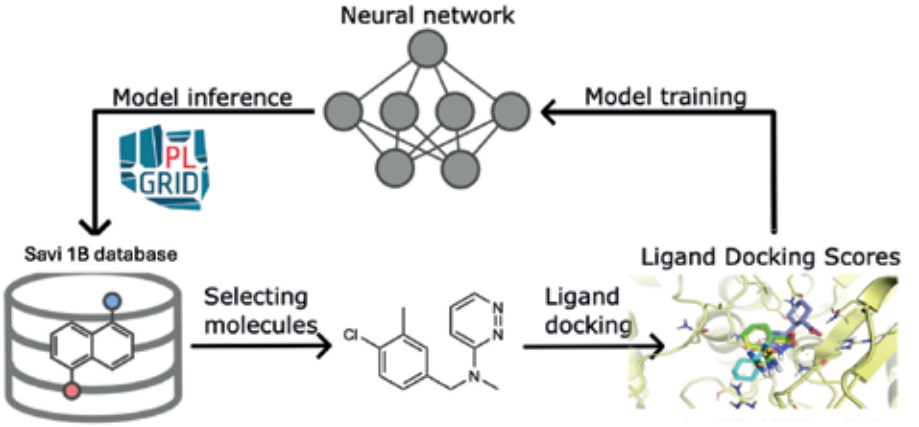

Fig.1. Workflow architecture for virtual screening with active learning.

5. Conclusions and future work

After docking ~3 M selected compounds (0.2% of the SAVI), the workflow successfully recovered most top-performing scaffolds that would otherwise require exhaustive enumeration. The approach preserved high scaffold diversity while prioritizing novel chemotypes. MC-Dropout effectively guided exploration toward sparse high-affinity regions, ensuring broad chemical coverage. Overall, this AL–driven virtual screening framework demonstrates that billion-scale structure-based discovery is achievable without full enumeration. By reducing docking volume by orders of magnitude while retaining hit quality and scaffold diversity, it provides a scalable strategy applicable across diverse molecular targets and docking platforms. In particular, the prioritized compounds will undergo experimental validation as potential inhibitors of LasR, a central virulence regulator and biofilm inducer in P. aeruginosa, supporting the search for novel anti-infective therapeutics.

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Oral presentation

Isolating Somatic Variants

Elżbieta Wierciak

AGH University of Science and Technology, al. Adama Mickiewicza 30, 30-059 Kraków, Poland

e.wierciak@gmail.com

Keywords: CLL, chronic lymphocytic leukemia, MBL, monoclonal B-cell lymphocytosis, scRNA-seq, single-cell RNA sequencing, computational medicine, bioinformatics

1. Introduction

The development of data and computer science opens exciting avenues for personalized medicine and disease prevention. An example of a disease that could be better understood with the support of computational methods is chronic lymphocytic leukemia (CLL) – the most commonly diagnosed blood cancer among European adults [1]. The exact cause of CLL is still unknown, but attempts to understand its genesis on a genetic level, as well as its connection to monoclonal B-cell lymphocytosis (MBL), have shown promise [2].

2. Description of the problem

Chronic lymphocytic leukemia affects B cells, causing them to multiply excessively and accumulate in the blood, bone marrow and lymphoid tissues, thus interfering with normal blood cell production and immune function [1]. Monoclonal B-cell lymphocytosis is a precursor condition to CLL characterized by the presence of small numbers of clonal B cells in the peripheral blood, but without the symptoms seen in full-blown leukemia [2]. In order to understand early CLL development, it is important to find out whether MBL drives the premalignant expansion or the malignant progression of CLL. To answer this question, genetic data from healthy subjects with MBL was sequenced using the Illumina scRNA-seq method. For each subject, each cell was tagged according to the clone it belonged to. The aim was to compare the genetic sequence of expanded clones against cells that do not belong to expanded clones. In order to avoid detecting genetic changes that are the result of inter-individual variability, each studied expanded clone and the reference non-expanded set were both sourced from the same individual.

3. Related work

A series of research that sparked the idea for this project was focusing on autonomous B-cell receptor signaling (BCR signaling) [3][4]. In this work it was shown that autonomous BCR signaling operates in MBL analogously to CLL. Subclonal genetic CLL driver mutations in MBL have also been observed [5], which would support the idea of gradual clonal expansion driven by moderate autonomous BCR signaling, potentially resulting in a level of genetic instability that facilitates graduate acquisition of CLL driver mutations.

4. Solution to the problem

Thanks to Cyfronet HPC resources and Leiden University Medical Centre, the scRNA-seq data was made available for analysis. Several methods of somatic variant detection were proposed and compared, then the best one selected. It involved creating a germline and expanded set count table, with the information for each position how many of each nucleotide were detected for both sets. Next a statistical test was carried out to determine what zygosity type each position in each set had. It was tested whether the

observed alternative reads can be explained by sequencing error (a fixed 5% error rate was assumed) or by a somatic variant, using a binomial likelihood. The GQ score was then used to measure the confidence with which the data supports the somatic variant hypothesis [5][6].

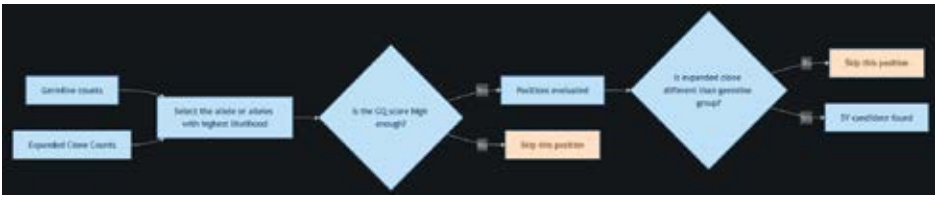

Fig.1. Diagram of the evaluation procedure.

5. Conclusions and future work

Several interesting somatic variant detection approaches were proposed for this problem based on previous similar work. Most genetic changes detected were losses of heterozygosity, and several SNPs were also detected. Insertions and deletions were beyond the scope of this work. Consultations with an immunologist are in progress to determine the impact of each of the detected somatic variants.

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Oral presentation

Explainable variational autoencoders for automatic annotation of hematopoietic stem and progenitor cells from scRNA-seq

Maja Błażejewicz

Jagiellonian University

maja.blazejewicz@student.uj.edu.pl

Keywords: scRNA-seq, hematopoietic stem cells, deep learning, variational autoencoder, explainable AI, cell type annotation

1. Introduction

Single-cell RNA sequencing (scRNA-seq) has become a transformative tool for understanding cellular heterogeneity, yet accurate cell type annotation remains a major challenge [1]. This is particularly evident in the hematopoietic system, where hematopoietic stem cells (HSCs) and progenitors represent a transcriptional continuum rather than discrete, easily separable populations. Traditional approaches have relied on surface markers such as CD34, which remain fundamental for defining HSCs. However, their expression is not strictly specific or stable, being influenced by environmental cues, cell cycle status, or metabolic changes.

2. Description of the problem

The limitations of classical marker-based annotation highlight the need for more robust computational strategies. scRNA-seq datasets capture high-dimensional gene expression profiles, offering opportunities to uncover subtle differences between closely related cell states. In hematopoiesis, precise discrimination between long-term repopulating HSCs, short-term progenitors, and lineage-committed cells is essential for understanding differentiation trajectories, aging, and hematological disorders [2]. Misclassification can distort biological conclusions, for example, by underestimating the frequency of highly regenerative cells or overestimating progenitor populations. The ability to identify subtypes with high resolution is therefore not only fundamental for basic research, but also has implications for transplantation, gene therapy, and clinical diagnostics. Additionally, it is crucial to understand how variability in gene expression translates into functional differences between closely related cell types and states, as this variability often underlies the trajectories of hematopoietic differentiation and disease progression.

3. Related work

Advances in machine learning, and deep learning specifically, have opened new possibilities for cell type classification in scRNA-seq. Methods such as random forest, gradient boosting, neural networks, and autoencoders can integrate information across thousands of genes, capturing relationships invisible to marker-based strategies. Among them, variational autoencoders (VAEs) provide a particularly powerful framework for modeling complex and continuous transcriptomic landscapes. Previous studies have demonstrated that autoencoder-based approaches can effectively reconstruct cellular trajectories and detect subtle transcriptional programs, extending beyond the resolution of classical clustering methods [3].

4. Solution to the problem

The use of VAEs combined with an explainable AI (XAI) framework enables both accurate annotation

and biological interpretability. By attributing gene-level importance scores to specific latent dimensions, XAI provides insights into the molecular features that drive differences between HSC subpopulations and along differentiation pathways. This interpretability bridges the gap between computational predictions and biological mechanisms, helping to identify transcription factors, regulatory programs, or stress-response genes that shape hematopoietic fate. Applied to scRNA-seq data, such models allow the mapping of trajectories with improved resolution while highlighting the gene expression signatures that underpin lineage priming and functional diversity within HSCs [4]ssumed) or by a somatic variant, using a binomial likelihood. The GQ score was then used to measure the confidence with which the data supports the somatic variant hypothesis [5][6].

5. Conclusions and future work

Integrating VAEs with explainability methods offers a powerful approach to refine cell type annotation in scRNA-seq, particularly for complex and heterogeneous systems such as hematopoiesis. Beyond automating and improving classification, this strategy provides mechanistic insights into gene programs defining stemness, differentiation, and disease states.

Future work will focus on validating the results across independent clinical datasets, extending the models to incorporate multimodal measurements, and deepening the biological interpretation of explainability outputs to better link computational findings with hematopoietic biology and disease mechanisms, further enhancing their relevance for translational hematology.

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Oral presentation

Analytical RVE theory of dispersed media and its applications

Vladimir Mityushev

Faculty of Computer Science and Telecommunications, Cracow University of Technology, Kraków, Poland

wladimir.mitiuszew@pk.edu.pl

Keywords: dispersed heterogeneous media, RVE, structural sums, classification of structures

1. Introduction

This note introduces an approach inspired by structural sums, which describes the interactions among inclusions of dispersed heterogeneous media. The structural sums serve as the cornerstone for mathematical models of random structures within the framework of the analytical Representative Volume Element (aRVE) theory. We quantified the inter-phase interactions within media and derived analytical formulas for their macroscopic properties. Application to the diagnosis and classification of glioma structures requires a set of corresponding pictures to develop the corresponding machine learning models, and can be performed together with the specialists in medicine.

2. Description of the problem

Gliomas, a type of brain and spinal cord tumor, are classified based on their cellular origin and molecular characteristics. The classification incorporates molecular data alongside traditional histological features and is based on simple observations and expert visual evaluations. This evolving understanding is necessary for the integration of molecular profiles into the diagnosis and classification of gliomas. Convolutional neural networks were introduced for automated, multiclass classification of glioma grades in [1]. This straightforward usage is based on the machine learning approach. It is supposed that the introduction of images and their corresponding deep processing by the almighty computer will lead to a result. The main difficulty for a wide application of the above approach is the huge number of features. On the other side, the fundamental characteristics of cellular dynamics can be locally approximated by diffusion, fluid transport, thermal conduction, and other chemo-physical processes within multiphase media. These phenomena are represented by systems of ordinary and partial differential equations from classical mathematical physics, such as the Laplace, Poisson, Navier–Stokes equations, and their coupled variants [2]. While this modeling framework yields insightful and generalizable results, its practical implementation typically relies on purely numerical solvers, which impose limitations due to high computational complexity and resource demands. The problem of essential reduction of the principal parameters becomes decisive in the considered problem of brain and spinal cord tumors classification.

3. Related work

Similar classification problems concerning dispersed composites have been studied for many years, beginning with Maxwell's and Rayleigh's works. Various approaches based on engineering observations, empirical models, and finite method simulations are very popular in material sciences. However, some analytical formulas were given without an analysis of their precision. This led, at most, to formally different but asymptotically equivalent formulas for the same classes of composites. Typical methods and tricks used by self-consistent methods and their modifications contradict the principles of homogenization and asymptotic models discussed in [3, Chapter 9] and

[4]. Randomness in composites is strictly related to the measure theory. In the considered case of non-overlapping inclusions, the measure theory is applied to the characteristic set equal to a tensor $\mathcal{E}_1$ in inclusions and to $\mathcal{E}2$ in the matrix. Theoretically, any such measurable set is determined by the infinite set of *n*-point correlation functions. Implementing multiple correlation functions for random composites is usually reduced to the well-studied spatial two-point correlation functions. Theoretically, the infinite set of multiple correlation functions completely describes a random composite. However, the virtual impossibility of computing the correlation functions of higher orders restricts their applications. A computationally effective method of structural sums was proposed in [5] and works cited therein. This method is based on the generalized Schwarz alternating method and the solution to the Riemann-Hilbert and $\mathbb{R}$-linear problems for an arbitrary multiply connected domain.

4. Solution to the problem

The approach described in [5] and works cited therein leads to the theory of *a*RVE. It can be considered a constructive application of the Decomposition Theorem [5]. One of the *a*RVE applications is outlined below. Let us have at our disposal two plane pictures of dispersed composites and their digital treatment in the form of two sets of the centers of inclusions, $\mathbf{a} = \{a_1, a_2, \ldots, a_N\}$ and $\mathbf{a'} = \{a'_1, a'_2, \ldots, a'_N\}$, scaled to the periodic unit square cell. We want to know whether these two media belong to the same class of random composites. First, we must calculate the structural sums described in [5] for two sets of points, a and a′, expressed by the vector sets $\mathbf{E} = \{e_1, e_2, \ldots\}$ and $\mathbf{E'} = \{e'_1, e'_2, \ldots\}$, and then compare them. The Decomposition Theorem [5] guarantees the complete geometric characterization of macroscopic properties of media represented by sets **a** and **a′**. The question of macroscopic anisotropy can be resolved by the same method.

5. Conclusions

The main advantage of aRVE compared to other methods can be summarized as follows:

- A class of random composites can be directly determined by a set of structural sums without the computation of its effective properties.
- The number of inclusions per periodicity cell is practically not restricted.
- The method doesn't use a virtually impossible computation of higher order
- correlation functions.

The derived theoretical model can be applied to the diagnosis and classification of gliomas. It requires a set of corresponding pictures to develop the corresponding machine learning models, and can be performed together with the specialists in medicine.

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Oral presentation

Enhancing neutron measurement techniques for heavy ion beam cancer therapy

Rafał Sawczyszyn[1,2], Leszek Grzanka[1,3], Jeppe Brage Christensen[2]

[1]AGH University of Krakow, al. Adama Mickiewicza 30, 30-059 Krakow, Poland
[2]Paul Scherrer Institute, Forschungsstrasse 1111, 5232 Villigen, Switzerland
[3]IFJ PAN, Walerego Eljasza-Radzikowskiego 152, 31-342 Krakow, Poland

rsawczyszyn@student.agh.edu.pl, jeppe.christensen@psi.ch, leszek.grzanka@ifj.edu.pl

1. Introduction

In particle therapy, precise dose delivery is essential for treatment efficacy and patient safety. Global use of proton and carbon ion therapy has risen rapidly, with over 300,000 patients treated [1]. However, therapeutic ion beams generate secondary neutrons that can deposit dose far from the target. Even low neutron exposures may increase long-term cancer risk, particularly in sensitive groups such as children and pregnant patients. This makes it particularly difficult to use radiation therapy with heavy ions to treat a tumor in the vicinity a critical organ or near the stomach of a pregnant patient.

2. Description of the problem

There does not yet exist a neutron detector to measure the neutron doses, which can be placed e.g. on the stomach of a pregnant patient. However, one candidate is track-etched detectors (CR-39), originally developed for neutron dosimetry in nuclear plants but the analysis algorithms—largely unchanged for 50+ years—lack modern computational methods and are highly sensitive to defects, noise, and damage. Machine learning offers the potential to greatly improve TED analysis, providing the accuracy and robustness needed for safe clinical implementation in particle therapy. We aim to improve the old detector system with modern machine learning to improve the patient safety during radiotherapy.

3. Related work

Recent studies in this field were carried out in 2025 in the United States. Machine learning was applied to the analysis of particles produced in deuterium–deuterium fusion reactions [3]. Specifically, scans from CR-39 detectors were analyzed using a compact neural network based on Ultralytics' YOLOv8 architecture. As a result, the network was able to successfully identify tracks left by proton and helium particle impacts. Different studies showed that machine learning methods can have high precision in track detection [4] [5].

4. Solution to the problem

To improve precision, we employed Mask R-CNN (Mask Region-based Convolutional Neural Network), introduced in 2017 by Facebook AI Research [2]. Mask R-CNN is a deep learning model designed for instance segmentation, meaning it can detect, classify, and separate individual objects within an image. By applying this approach to detector scans, the network can more accurately distinguish meaningful structures from defects or noise, significantly improving the reliability of the analysis. Our dataset consists of approximately 12,000 detector scans, each corresponding to known radiation doses.

Neural network is trained on PLGrid High Performance Computing cluster (HPC) - Athena. This allows us to rigorously evaluate the network's accuracy and identify possible improvements in detection performance.

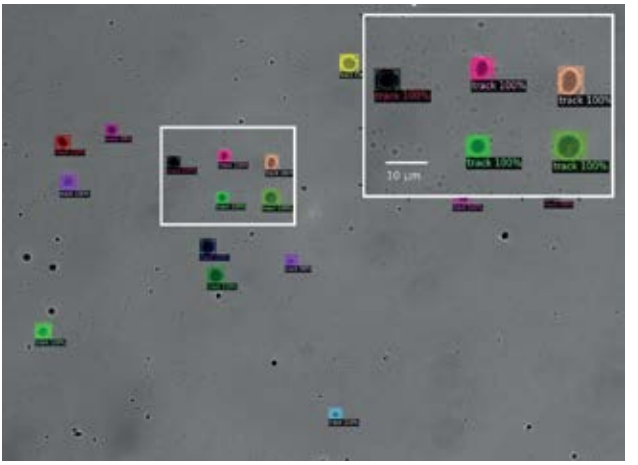

Fig.1. Tracks detected on a heavily damaged CR-39 detector using Mask R-CNN.

5. Conclusions and future work

The current approach is effective, allowing us to identify over 85% of the tracks in an image. This means that a therapy plan with heavy ions can be experimentally validated, when the images are evaluated with the developed algorithm. In turn, this may reveal if a treatment will cause a large neutron dose to a critical region such as the stomach of a pregnant patient.

Future work will focus on further optimizing these elements, expanding the dataset with more diverse detector scans, and refining the network architecture to improve precision and robustness in detecting particle tracks.

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Oral presentation

CT-based heart digital twin can improve estimation of vectorcardiographic derived positions of the electrical activity

Michał Szafarczyk, Krzysztof Malinowski, Sandra Zarychta, Julia Kolasa, Klaudia Proniewska, Peter van Dam

[1]Center for Digital Medicine and Robotics, Jagiellonian University Medical College, Krakow, Poland
[2]Laboratory of Functional and Virtual Medical 3D Imaging – 3D-FM, Department of Diagnostic Imaging, University Hospital in Krakow, Krakow, Poland

michal.szafarczyk@student.uj.edu.pl

1. Introduction

The electrocardiogram (ECG) is one of the oldest electrical measurements of the human body and provides instant information on the cardiac function as well as mechanical or structural changes in the heart. The vectorcardiogram is a related tool that represents electric activity as the direction of a vector and the average cardiac anatomical location of activation over time [1].

2. Description of the problem

Although ECG contains information on heart anatomy as waveforms are majorly determined by the 3D shape of the heart in relation to the electrodes, creation of the average cardiac anatomical location of activation is based on underlying assumptions on the heart model and orientation as well as torso model and electrode placement. Contrary to ECG which is patient-specific, remaining models (heart, torso, electrodes) are generic.

Providing personalized, patient specific heart, torso and electrode placement models can facilitate estimation of the average cardiac anatomical location of activation and further improve its diagnostic performance in detection of abnormal ECGs. One readily available source of such information can be Computed Tomography (CT) scans.

3. Related work

It has been shown that vectorcardiographic derived positions of the electrical activity (PathECG) as well as waveforms (WaveECG) can be used in rapid identification of ECG abnormalities [2][3].

Digital twin technology has proven to be a great approach for many tasks in the medical field [6]. On top of that, it's a way in which medicine becomes more personalized and patient oriented.

Medical imaging data, besides being by itself a modality very useful for diagnostics, has also been shown to be a great tool for enhancing other diagnostic methods. MRI and CT scans have already been used in generating more accurate 3D heart models for electrophysiological simulations [7], creating highly personalized heart models for SCD risk assessment [8] or generating reconstructions of aortic valve for calcification quantification [9].

4. Solution to the problem

Estimated from CT:

- chest depth and width at position heart (to estimate chest dimensions)
- estimate heart position and orientation.

These parameters can then be used by CineECG to adapt the torso and heart model to compute a more patient specific PathECG [4][5].

5. Conclusions and future work

This research presented a novel method of injecting additional patient-specific information to the creation of vectorcardiogram-derived PathECG based on CT scans. However, only chest dimensions and heart position and orientation were used. The presented method will be further improved to develop a full patient specific heart and torso model including actual lead placement in order to maximize the diagnostic performance of methods using PathECG to identify ECG abnormalities.

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