# AIME21

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# Book of Abstracts

AIME20
Book of abstracts

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**1**

# Opening

Opening
Dr. Péter Lévai
Director General
WIGNER RCP

**2**

# Superfeminine and Supermasculine Connections of the Human Brain

**Authors:** Vince Grolmusz[None]; Laszló Keresztes[1]; Evelin Szögi[1]; Bálint Varga[1]

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The anatomical network of the human brain is one of the most complex and most intriguing object of study the humanity may encounter today. We demonstrate an Artificial Intelligence-based method, which is capable of identifying the most relevant brain connections, which define the sex of the subject. The work is based on the largest and the highest quality braingraph collection to date, the https://braingraph.org 1054 robust collection of connectomes, using the dMRI data of the NIH-funded Human Connectome Project.
Our most surprising result is the identification of 2 superfeminine and 3 supermasculine connections of the brain, which determine the sex of the subject if they are strong or weak enough, independently of the other connections of the brain.

**authors**:

Keresztes, László;Szögi, Evelin; Varga, Bálint; Grolmusz, Vince

**Title**:

Superfeminine and Supermasculine Connections of the Human Brain

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**3**

# Hardness of planning and learning with linear function approximation in reinforcement learning

**Authors:** Csaba Szepesvari[1]; Gellert Weisz[2]; Philip Amortila[3]

[1] *DeepMind/University of Alberta*

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Markov decision processes (MDPs) is a minimalist framework that is designed to capture the most important aspects of decision making under uncertainty, a problem of major practical interest. Unfortunately, the price of the minimalist approachis that MDPs lack structure and as such planning and learning in MDPs with combinatorial-sized state and action spaces is strongly intractable. An appealing idea to overcome this intractability is to assume that the optimal action-value function, which effectively captures everything that needs to be known about an MDP in order to act optimally in it, enjoys some distinct structural properties, such as that it can be written as the linear combination of a tractable number of basis functions. The question is whether this structure is sufficient to design algorithms that overcome the inherent intractability of planning and learning in MDPs. In this talk, I will look back at research addressing this question (starting in the 1960s) and then present a recent result that shows that the MDP planning and learning problems remain strongly intractable even with the extra assumptions, as far as scaling with the planning and the number of basis functions is concerned. I will finish with listing a number of open problems.

**authors**:

Weisz, Gellert; Amortila, Philip; Szepesvári, Csaba

**Title**:

Hardness of planning and learning with linear function approximation in reinforcement learning

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## Playing detective: Dissecting silent failures of Deep Learning models for 3D Point Clouds

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Silent failure effects in Deep Learning models are challenging, to say the least. Image processing applications have developed various tools in order to help explainability and debugging, including visualizign kernel activations, heat maps, and so on. Learning on 3D point clouds is especially challenging as we deal with an unstructured data of a point set defined in 3D metric space. Models operating on this native format face multiple challenges compared to models working on images, including rotation and permutation invariance.
This talk will show an example of a silent failure in a 3D point cloud model and the detective work done in order to decode and understand its inner workings. Following a rigorous approach helps us draw the right conclusions as well as aid us in deciding where to start the re-design.

**authors**:

Robert-Zsolt Kabai

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Team Lead, Deep Learning for Point Cloud

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## nucleAIzer: nucleus segmentation with DL & image style transfer

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Cellular analysis based on microscopy images starts with the identification of cells, typically by segmentation. This challenges researchers to construct out-of-the-box solutions that potentially work in various experiments as downstream analysis depends on segmentation reliability. nucleAIzer is a deep learning-based pipeline intended for the efficient and robust instance segmentation of cellular compartments, even on such new image modalities for which no ground truth data is available by adaptation to them via image style transfer learning. With this technique we can generate synthetic images in the new, unknown experiments' domain and forward this information to the training of a segmentation model, thus preparing it to cope with such images.

**authors**:

Reka Hollandi1, Abel Szkalisity1, Timea Toth1,2, Ervin Tasnadi1,3, Csaba Molnar1,3, Botond Mathe1, Istvan Grexa1,4, ..., Ferenc Kovacs1,8, Lassi Paavolainen7, Tivadar Danka1, Andras Kriston1,8, Anne Elizabeth Carpenter6, Kevin Smith9,10, Peter Horvath1,7

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**6**

## Market liquidity, order book dynamics and machine learning

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Trading in financial exchanges is becoming increasingly data driven and algorithmic due to the large amount of detailed data available about the limit order book and the increasing speed competitive nature of trading. I will argue that because of this, algorithmic trading is a great playground for machine learning methods.
In this talk I will discuss what kind of real-life data science problems we faced with in a machine learning based trading team. To put the business problem in context I will first talk about the different participants in a financial exchange. We will also briefly discuss how traders interact with the limit order book and what is the role of liquidity and market makers. I will then describe the type of big data which describes the order book dynamics, the different approaches one can take, and learning algorithms one can use when designing market making trading algorithms.

**authors**:

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## Machine Learning in Government Bond Trading

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Government bond trading is going through unprecedented change today, the role of traditional (mostly voice broking) bond trading model is decreasing due to the electrification of the markets.
The electrification means more reliable and good quality data that give a solid foundation to the application of advanced statistical approaches.
Our aim is to highlight applications in bond trading from pricing to order execution through alpha signal generation where machine learning techniques offer improvements.

**authors**:

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Machine Learning in Government Bond Trading

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**8**

## Taming neural networks with TUSLA: Non-convex learning via adaptive stochastic gradient Langevin algorithms

**Authors:** Attila Lovas[1]; Miklós Rásonyi[1]; Iosif Lytras[2]; Sotirios Sabanis[2]

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Artificial neural networks (ANNs) are typically highly nonlinear systems that are finely tuned via the optimization of their associated, non-convex loss functions. Typically, the gradient of any such loss function fails to be dissipative making the use of widely-accepted (stochastic) gradient descent methods problematic. We offer a new learning algorithm based on an appropriately constructed variant of the popular stochastic gradient Langevin dynamics (SGLD), which is called the tamed unadjusted stochastic Langevin algorithm (TUSLA). We also provide a non-asymptotic analysis of the new algorithm's convergence properties in the context of non-convex learning problems with the use of ANNs. Thus, we provide finite-time guarantees for TUSLA to find approximate minimizers of both empirical and population risks. The roots of the TUSLA algorithm are based on the taming technology for diffusion processes with superlinear coefficients as developed in Sabanis (2013, 2016) and for MCMC algorithms in Brosse et al. (2019). Numerical experiments are presented which confirm the theoretical findings and illustrate the need for the use of the new algorithm in comparison to vanilla SGLD within the framework of ANNs.

**authors**:

Attila Lovas, Miklós Rásonyi, Iosif Lytras, Sabanis Sotirios

**Title**:

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**9**

## Methods for Interpreting Text Autoencoders

**Authors:** Bálint Gyires-Tóth[1]; Marco H A Inácio[None]

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Calculating text statistics, like term frequency and similarity is an essential part of processing and modeling symbol sequences, including, for instance, text, source codes, and DNA sequences. However, calculating these statistics may have high computational demand. Thus, even in case of datasets with a moderate size, it can be cumbersome to integrate it into research or commercial product. As the size of the dataset increases, it can even become unfeasible. Therefore, surrogate models can be trained to approximate these statistics - directly with supervised learning, or indirectly with self-supervised approaches.
In this talk, a novel method is introduced for analyzing text autoencoders in terms of reconstruction loss and learned representation in the bottleneck. The method utilizes the reconstruction loss of the autoencoder to approximate text statistics, like term frequency and other string similarity metrics (including Levenshtein Distance and Longest Common Subsequence). The performance of convolutional neural network and Long Short-Term Memory-based autoencoders are investigated on public datasets (Penn Treebank, DBpedia, Yelp Review Polarity).
The results help to interpret what text autoencoders learn. It is also a step towards understanding what properties might be represented in text embeddings.

**authors**:

Bálint Gyires-Tóth, Marco H A Inácio

**Title**:

Methods for Interpreting Text Autoencoders

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**10**

## VPNet: Variable Projection Networks

**Authors:** Sándor Fridli[1]; Péter Kovács[1]; Gergő Bognár[1]

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Analysis of signals by means of mathematical transformations proved to be an effective method in various aspects, including filtering, system identification, feature extraction, classification, etc. The most widely used method in transform-domain techniques operates with fixed basic functions like trigonometric functions in the Fourier transform, Walsh functions in Walsh–Fourier transform, mother wavelet function for wavelet transforms, etc. In these cases, the flexibility of the method is in the proper choice of the function system. Once the system is set it is used regardless the difference between the individual signals. In other words, the system can be adjusted on the problem level, but not on the individual signal level. This limitation turned to be significant, especially in dynamically changing environments, when we need to adjust the system to the signal. One way to surpass this limitation is to use adaptive orthogonal transformations. In recent years, we generalized this concept, developed various adaptive mathematical models, and successfully applied them in a range of applications, including ECG, EEG signal processing, telecommunication, CT-, photoacoustic-, and thermographic imaging. In these applications the transformation step was followed by machine learning techniques. Even though the interaction of these two phases were studied and considered they were not integrated into a uniform method. In our recent project, based on our former work, we incorporate the representation abilities of adaptive orthogonal transformations and the prediction abilities of neural networks (NNs) in form of the model called VPNet. This is a novel model-driven NN architecture for 1D signal-processing which utilize variable projection (VP). Applying VP operators to neural networks has the advantage of learnable features, interpretable parameters, and compact network structures. We show that, compared to fully connected and one-dimensional convolutional networks, VPNet offers fast learning ability and good accuracy at a low computational cost of both training and inference.

**authors**:

Péter Kovács, Gergő Bognár, Sándor Fridli

**Title**:

VPNet: Variable Projection Networks

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## Two years into the ESS Control System Machine Learning Project

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The European Spallation Source ERIC (ESS) is a joint European organisation committed to building and operating the world's leading facility for research using neutrons. The facility design and construction includes a powerful linear proton accelerator, a helium-cooled tungsten target wheel and two dozen state-of-the-art neutron instruments.

ESS is made up of a large number of diverse systems and disciplines, covering for example water cooling, vacuum, power distribution, timing systems, information technology, networking, microwaves, cryogenics among others. These systems are integrated and controlled by the central integrated control system (ICS), which acts as the "brain" of the ESS machine.

The ESS machine will generate at least an order of magnitude larger volumes of control system related data than typically existing in large industries. With an estimated number 100 000 devices to

control and 1.6 million process values in the control system we realize that the high-level requirement of 95% availability for the facility will be very challenging and that ICS will play a key role to reach this goal. For this reason, ESS initiated a control system machine learning (CSML) project in 2018. The project will explore how application of modern machine learning technologies to a large-scale industrial distributed control system can help increase facility availability and efficiency and lower costs for operation.

This talk will cover the activities and outcome of the two first years in the project.

**authors**:

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**12**

## Insights to Hit to Lead

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The work discussed here is in progress nevertheless it provides insights into good practices in drug design, discovery, and development (4D). The final goal is to make the 4D flexible and scalable and reduce the total time for bringing a new chemical entity to the market a few times. The focus of the presentation is on bio-chemistry data, its discretization, augmentation, and saturation (DAS). The digital twin approach has been employed for domain digitalization. The idea behind is to use GOAL oriented approach to represent the objectives that may vary or change over time in order to achieve the final goal in 4D. It is a belief of the team behind this work that 4D needs to handle adequately the dynamically changing environment and any new piece of knowledge need to be explored. The emphasis presented here in the 4D process is on the AI pipelines and processes that allow prediction of chemical properties and how this information is used to generate virtual libraries that facilitate the establishment of drug candidates and reduce the choice of stem molecules from a few thousand or millions to a hand full. The software at the end is presented as a SaaS and a PaaS is used for implementation.

**authors**:

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**13**

## Hastlayer - Implementing on Xilinx Alveo Accelerator Cards

**Authors:** Erno David[1]; Dávid El-Saig[2]; Zoltán Lehóczky[2]

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Hastlayer (https://hastlayer.com/) by Lombiq Technologies is a .NET software developer-focused, easy to use high-level synthesis tool with the aim of accelerating applications (possible areas include AI/ML, image/video processing, scientific computations…). It converts standard .NET Common Intermediate Language (CIL) bytecode into equivalent Very High Speed Integrated Circuit Hardware Description Language (VHDL) constructs which can be implemented in hardware using FPGAs. One such available target FPGA platform is the Xilinx Alveo Data Center accelerator card family which will be soon deployed in the major cloud-based data centers. This talk presents an overview of how Hastlayer integrated with the Xilinx framework

**authors**:

Ernő Dávid, Dávid El-Saig, Zoltán Lehóczky

**Title**:

Hastlayer - Implementing on Xilinx Alveo Accelerator Cards

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**14**

## Conversational AI Technology - Business Applications

**Authors:** Nadia Kaloyanova[None]; Martin Minchev[None]

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We are a company from the private sector and we can share our experience on what are the most common business applications of our (and in general) AI Conversational Technology and Natural Language Understanding.

Some of the most common use cases for our technology are:

- Deep Sentiment and Opinion Analysis - extract content from pdf files, web articles and video files, and analyze it to extract key topics, opinion holders, opinion targets, and sentiment expressions.
- AI Knowledge Base - using AI to transform static guides and documentation into an interactive knowledge base that provides answers to a specific user questions.
- AI Reporting - analysing data and producing on demand real time reporting for employees. E.g. The employee asks “What were our sales last month” and the AI analyses the data and gives the concrete answer “The sales for last month were 3 mln” rather than the employee having to read the sales reports and calculating it
- AI Assistants for Customer Support, making handling customer requests more efficient and helping agents be more effective. The Customer Support can also be integrated with social media channels such as Twitter, Facebook, Skype and Slack.
- Using an AI Assistant internally to automatically assign incoming customer requests/emails to the right department and monitoring the sentiment about KPIs in real time

- Easier internal case raising and updating - the AI Assistant can be integrated with the company's back-end systems and provide an easy to use interface to the employees, helping them managing tickets/cases, rather than the time consuming logging into systems like MS Dynamics, Salesforce, etc. which are confusing, difficult to use, people miss steps, etc.

**authors**:

Nadia Kaloyanova and Martin Minchev

**Title**:

Conversational AI Technology - Business Applications

**affiliation**:

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**15**

## Considerations and Applications for HPC, Machine Learning and AI technologies for accelerating scientific discovery at next generation research infrastructures.

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Research infrastructures (RI) provide access to state-of-the-art instrumentation for the scientific community for example, The Extremely Brilliant Source at the European Synchrotron Radiation Facility, the European Free Electron Laser and the European Spallation Source.
The business case for these facilities is centred on a service model that provides visiting researchers access to cutting edge scientific instrumentation and methods, enabling accelerated delivery of high impact science.
Neutron and photon RIs share a number of key commonalities which present certain challenges that must be addressed to ensure that the RI business model is efficient.

• Data rates and experimental data volumes are challenging for users and facilities.
• High data rates enable complex experimental studies in real (or near real) time. Kinetic studies of reactions or phase transitions result in data collected at rate that challenges experimental teams' ability to steer the experiment in a considered.
• Neutron and photon methods provide unparalleled insight into physics at the atomic scale. Analysis of data requires the use of modelling and simulation tools that are from a theoretical standpoint state of the art, requiring dedicated HPC environments and expertise.
• The research community leverage the complimentary of photon and neutron research methods, creating a need for interoperable data and data services for facility users.

Leveraging HPC is an essential ingredient for enabling scientific impact, these challenges will be discussed in the context the current status and strategy for high performance computing.
Machine learning and artificial intelligence technologies are seen as a future key enabler for experimental methods and scientific computing that could provide specific solutions for our key challenges of data rate and real time processing these will be discussed within the context of the important scientific consideration of trust and reproducibility.

**authors**:

Jonathan Taylor

**Title**:

Considerations and Applications for HPC, ML/AI at next generation research infrastructures

**affiliation**:

European Spallation Source ERIC

**16**

## Representation and control: linear or nonlinear dimensionality reduction?

**Author:** Sandro Mussa-Ivaldi Mussa-Ivaldi[1]

[1] *Northwestern University*

Divide et impera – divide and rule – is an ancient political strategy broadly applicable to complex problems. Theoretical considerations and experimental evidence suggest that this is how the nervous system generates full repertoires of actions by the combination of pre-defined actions or policies. In the framework of geometry, the linear combination of basis vectors spans a vector space. There is empirical evidence that this geometrical view may be consistent with the way the neuromuscular system generates and combines mechanical forces. A similar view has been proposed to represent the kinematics of hand actions through the linear combination of few principal components. I will discuss some recent findings that cast doubts on the latter linear approach suggesting that the kinematics of gestures and hand actions have latent manifolds with significant nonlinear structure. The use of nonlinear methods for dimensionality reduction is however a mixed blessing: as one may gain higher fidelity in movement representation, abandoning linearity comes at the cost of greater complexity in control. I will discuss how the use of cartographic techniques may shed light on this tradeoff.

**authors**:

**Title**:

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**17**

## The Hungarian AI strategy

**Author:** László Boa[1]

[1] *Technical Coordinator Hungarian National AI Coalition The Hungarian AI strategy 2020-2030*

In this talk, I present the key institutional background and projects of Hungary's AI strategy. The goal of the Strategy is to harness the possibilities inherent in technological change and maximize the opportunities offered by artificial intelligence (AI). The strategy was prepared with the involvement of over 250 member organizations of Hungary's AI Coalition and over a thousand experts identified focus areas and highlighted projects.

As part of the Strategy, the National Data Asset Agency was established, which manages and controls access to governmental data. Two Transformative Projects have already started the implementation. The Governmental Chatbot project aims to automate 60% of government office

services. And in the Data Valet project, a service will be developed for the citizens to control access rights of their personal data to be used in public and private AI applications. More transformative projects will be initiated, for instance, to control irrigation in agriculture. AI is expected to add 11-14 percent to Hungary's GNP by 2030.

**authors**:

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**18**

## The first year of the Hungarian Artificial Intelligence National Laboratory (MILAB)

**Author:** András Benczúr[1]

[1] *Scientific director Artificial Intelligence National Laboratory Institute for Computer Science and Control (SZTAKI)*

With the goal of strengthening Hungary's position in AI, MILAB is founded in 2020 as the coordinated national artificial intelligence umbrella for the collaboration of all major research centers, universities and large-scale national programs. With the participation of 75 researchers, we established a project structure of six main areas during the kickoff meeting on September 2:
- Foundations of AI: bridging the gap between mathematical theory and machine learning practice.
- Human Language Processing: automating speech and text-based interactions, with Hungarian as primary focus.
- Machine perception: interpreting and organizing information coming from distributed multimodal sensors.
- Medical, Health and Biology
- Security and Privacy: eliminating the failures of AI systems by creating transparent, verifiable, explainable machine learning models; devising privacy preserving data sharing and analysis methods.
- Sensors, IoT and Telecommunications: capitalizing on the promise of big data, by transforming massive datasets into newfound knowledge that will enable timely data-driven decision-making and lead to new business opportunities.
You may join the active research life, the regular online events at https://milab.hu/

**authors**:

**Title**:

**affiliation**:

**19**

## Welcome

Dr István Szabó
ELKH
Secretary General

**20**

# Life beyond the pixels: single-cell analysis using machine learning and image analysis methods

**Author:** Péter Horvath[1]

[1] *BRC Szeged, Hungary*

In this talk I will give an overview of the computational steps in the analysis of a single cell-based large-scale microscopy experiments using deep learning techniques. First, I will present a novel microscopic image
correction method designed to eliminate illumination and uneven background effects. New single-cell image segmentation
methods will be presented using differential geometry, energy minimization and deep learning methods (www.nucleaizer.org). I will discuss the Advanced Cell Classifier (ACC) (www.cellclassifier.org), a
machine learning software tool capable of identifying cellular phenotypes based on features extracted from the image. It provides an interface for a user to efficiently train machine learning methods to predict various phenotypes. For cases where discrete cell-based decisions are not suitable, we propose a method to use multi-parametric regression to analyze continuous biological phenomena. To improve the learning speed and accuracy, we propose an active learning scheme that selects the most informative cell samples.
Our recently developed single-cell isolation methods, based on laser-microcapturing and patch clamping, utilize the selection and extraction of specific cell(s) using the above machine learning models. I will show that we successfully performed DNA and RNA sequencing, dPCR, and targeted electrophysiology measurements on the selected cells.
Finally I will show our results in the COVID-19 fight using deep learning methods (Daly etal Science).

**authors**:

**Title**:

**affiliation**: