
One-off

Realized

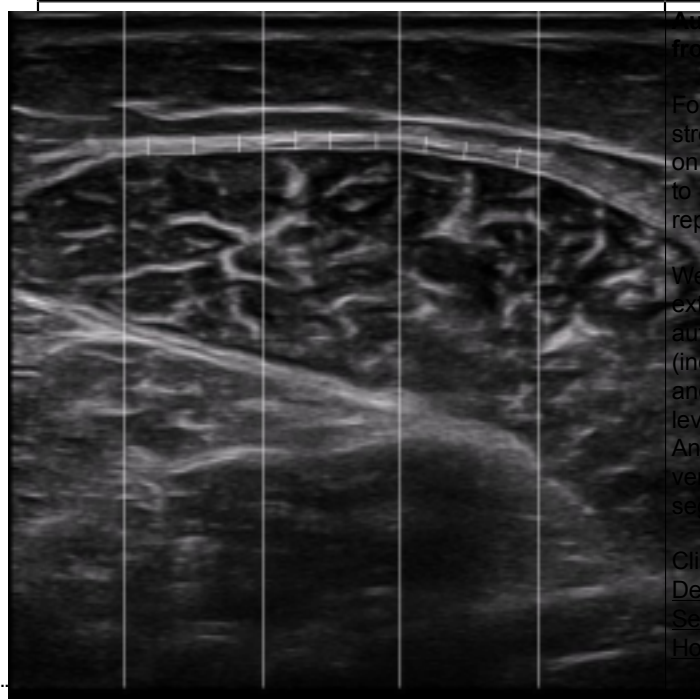
	Deployment of NEST Teaching Software on a Faculty HPC Cluster For Karolína Korvasová and the course Introduction to Computational Neuroscience at the Faculty of Mathematics and Physics, Charles University, we delivered the deployment and integration of the NEST Desktop and NEST Simulator software into the faculty's HPC infrastructure. The solution enables students to work with both a graphical user interface and Jupyter notebooks directly on the university HPC cluster, without reliance on external European research infrastructures. The work included integration with JupyterHub, operation via SLURM, containerization using Apptainer, modifications of the proxy layer, and resolution of security and XSRF-related issues in the communication between NEST Desktop, NEST Server, and JupyterHub. Client: Karolína Korvasová, M.Sc., Dr. rer. nat., Computational Systems Neuroscience Group MFF CUNI
	Running Origin Software on Linux for Scientific Data Analysis For Department of Condensed Matter Physics, we addressed the challenge of using the analytical software Origin in a Linux environment, which is commonly recommended for scientific work and access to HPC clusters, despite the fact that the software does not provide a native Linux version. The goal was to enable Linux users to perform full-featured data analysis while maintaining compatibility with existing projects and collaboration across research groups. Client: doc. RNDr. Karel Carva, PhD., Department of Condensed Matter Physics MFF CUNI
	Containerization and Easy Installation of GBTolib and UKRmol+ For Zdeněk Mašín's team, we prepared a distribution of computational codes GBTolib and UKRmol (UKRmol-in/UKRmol-out) to make them usable even for users without experience in compilation and linking. The goal was to remove the barrier of complex builds (BLAS/LAPACK, OpenMPI, SCALAPACK/ELPA, etc.) and deliver a reproducible environment for release.

	We delivered (1) a build via Conda/Mamba including CI adjustments on GitLab and supplemented documentation, and (2) ready-made containers (Docker ? Apptainer) suitable for operation on the Chimera cluster, including instructions for running via SLURM. The work also included ensuring dual compilation (double + quad precision) and a testing workflow using ctest. Client: Mgr. Zdeněk Mašín, Ph.D., Institute of Theoretical Physics, MFF CUNI
	Data Processing and Analysis of Single-Cell Gene Activity For Adam Klocperk's team, we processed experimental data from a modern method that tracks gene activity in individual cells. The original data contained several technical issues (poorly matched samples, missing patient labels, a portion of low-quality cells) that needed to be corrected first. We performed comprehensive data cleaning, removal of low-quality cells, and subsequent cell assignment to actual patients using genetic information. Data from different measurements were integrated to enable meaningful comparison, and we automatically classified individual cells by type (e.g., various T lymphocyte subtypes). The result is a well-processed dataset prepared for biological interpretation and further research. The project also included the creation of an internal tool (AI assistant) that helps with analysis preparation and technical report generation. Client: doc. MUDr. Adam Klocperk, Ph D., Department of Immunology, Second Faculty of Medicine, CUNI
	Web Interface for Risk Analysis (CLIP) For the CLIP team, we created a simple web interface for monitoring risk development over time. Users upload evaluated risk tables (FMEA) for individual years (e.g., 2024, 2025, 2026) into the application, and the system automatically displays clear graphs showing changes in risk levels over the years. The goal was to replace manual work with spreadsheets and graphs and enable quick and clear evaluation of trends. The application is designed so that non-technical users can also use it, and it is available in Czech according to the client's requirements. Client: Mgr. Jan Stuchlý, Ph.D., Childhood Leukemia Investigation Prague (CLIP)
	AI pipeline for processing medical reports We developed an AI tool to transform specialized medical reports into clear, understandable Czech for patients. The system operates as a pipeline: the input is the original medical text, and the output is a structured, linguistically simplified summary while preserving factual accuracy. The solution combines an extensive knowledge base (ICD-10, drug databases, abbreviations, etc.) with a



term-matching algorithm (Aho–Corasick) and the large language model Qwen2.5 for text generation. We use few-shot prompting and controlled generation parameters to improve output consistency. The goal was to create a containerized service ready for on-premise deployment in healthcare environments, with an emphasis on expanding the knowledge base and expert validation of outputs.

Client: doc. RNDr. Karel Fišer, Ph.D. Second faculty of medicine CUNI



Automation of Deep Fascia Thickness Measurement from Sonographic Images

For the Rehabilitation Clinic, we are developing tools to streamline the measurement of deep fascia thickness on ultrasound (sonographic) images. The project aims to reduce time consumption, increase measurement reproducibility, and minimize subjective operator influence.

We are developing two solutions in parallel. The first extends ImageJ with a custom macro and implements automated thickness calculations from a prepared mask (including variants based on distance transform, skeleton, and perpendicular cross-sections). The second solution leverages modern segmentation models such as Segment Anything Model (including experiments with the SAM3 version and medical adaptations) for semi-automatic fascia segmentation directly from unlabeled images.

Client: Mgr. Adéla Quittková,
Department of Rehabilitation and Sports Medicine at Second Faculty of Medicine CUNI and Motol University Hospital

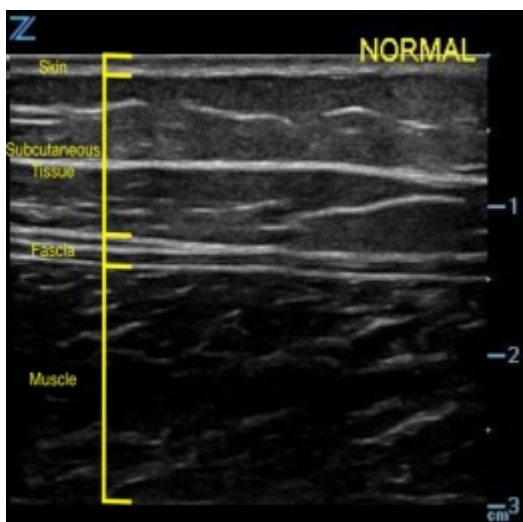


Secure Deployment of Sensitive Cloud for Processing Sensitive Data

We are preparing a workflow for the team of Jakub Drápal to preprocess sensitive legal data in the Sensitive Cloud environment, ensuring that raw data remains in isolation (read-only) and only approved, anonymized outputs leave the system.

A key component is the offline distribution of R and Python environments: we assemble and test complete library sets outside the cloud (conda-lock/CI), prepare them as read-only archives (conda-pack), and deploy them to Sensitive Cloud as pre-built versions without the possibility of ad-hoc installations. This also includes setting up the user desktop (RStudio/Jupyter/VS Code) and implementing secure data transfer via S3, along with an approval workflow.

	Client: doc. JUDr. Jakub Drápal , M.Phil., Ph.D., <u>Faculty of Law, CUNI</u>
	Web Platform for Vojta Method Study (SymBaby) For the Rehabilitation Clinic of the 2nd Faculty of Medicine, Charles University and Motol University Hospital, we are designing and developing a web platform for a multicenter study of Vojta method therapy. The system should enable collection and management of sensitive data across multiple sites while maintaining GDPR requirements, auditability, and secure data storage. We are preparing an application prototype with forms, user management, and change logging, including architecture design that allows physical data storage at Motol University Hospital and controlled access for external sites. The project also includes solutions for future deployment (inspired by the REDCap platform) and clarification of the operational model and infrastructure responsibility. Client: Mgr. Adéla Quittková, <u>Department of Rehabilitation and Sports Medicine at Second Faculty of Medicine CUNI and Motol University Hospital</u>
	Implementation of WGS Pipeline into TSPS We are expanding the Triple S Pipeline System (TSPS) with a complete workflow for whole-genome sequencing (WGS) analysis based on methodology published in <u>Nature</u> . The goal is to integrate dozens of specialized bioinformatics tools (e.g., BWA-MEM, Mutect2, Manta) into a single automated and reproducible process. The pipeline processes raw sequencing data, identifies genetic variants (point mutations, large-scale genomic rearrangements), evaluates their significance, and produces clear outputs for further biological or clinical interpretation. The result is a scalable infrastructure that enables reliable analysis of large genomic datasets without manual orchestration of individual steps. Client: Mgr. Jan Stuchlý, Ph.D., <u>Childhood Leukemia Investigation Prague (CLIP)</u>
	Autotracking of Aponeurosis Slip in Calf Muscle For a research team in the field of rehabilitation, we are developing a tool for automatic tracking of upper and lower muscle layer (aponeurosis) movement from ultrasound video. Currently, movement is evaluated through manual tracking of a single point on each layer frame by frame, which is very time-consuming and imprecise. The goal is to create a semi-automated software that enables tracking of multiple points simultaneously or analyzing the motion of entire regions using optical flow methods (e.g., Lucas–Kanade method or Farnebäck). The output is a quantitative description of the relative motion



between both layers, which can serve as a biomarker for research and potential future clinical diagnostics.

Client:

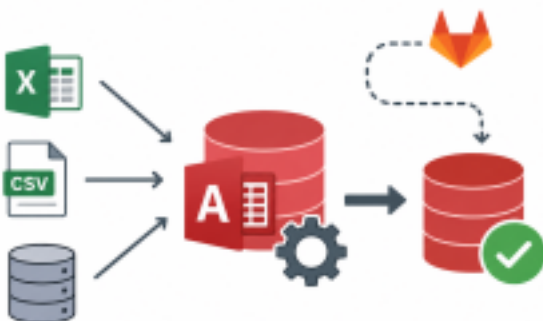
Mgr. Jakub Jačisko,
Department of Rehabilitation and Sports Medicine at
Second Faculty of Medicine CUNI and Motol University
Hospital



Web Interface for Exploring Egyptology Data

This project focuses on developing a web interface for exploring a curated dataset on the representation of women in ancient Egypt, currently containing over 2,100 manually verified records. The interface provides simple full-text search and column-based filtering, making the data accessible to researchers and students without requiring SQL knowledge. The data are hosted by Charles University and are planned to be expanded in the future. The platform offers a flexible tool for teaching and research in Egyptology and allows for the potential integration of additional records and advanced queries.

Client: Susan Anne Kelly, Ph.D. Czech Institute of
Egyptology at Faculty of Arts CUNI



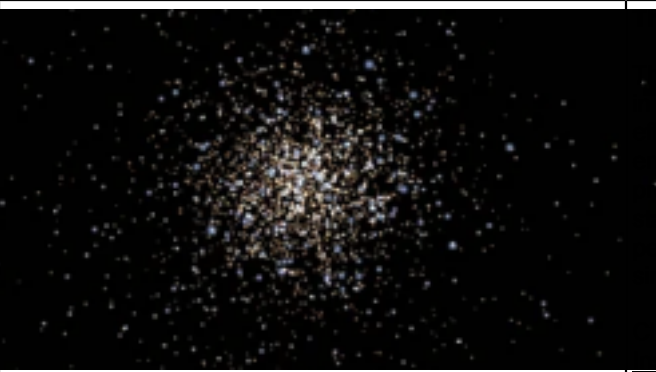
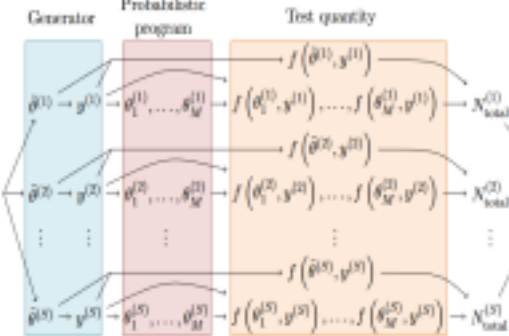
Processing of medication data updates in Microsoft Access

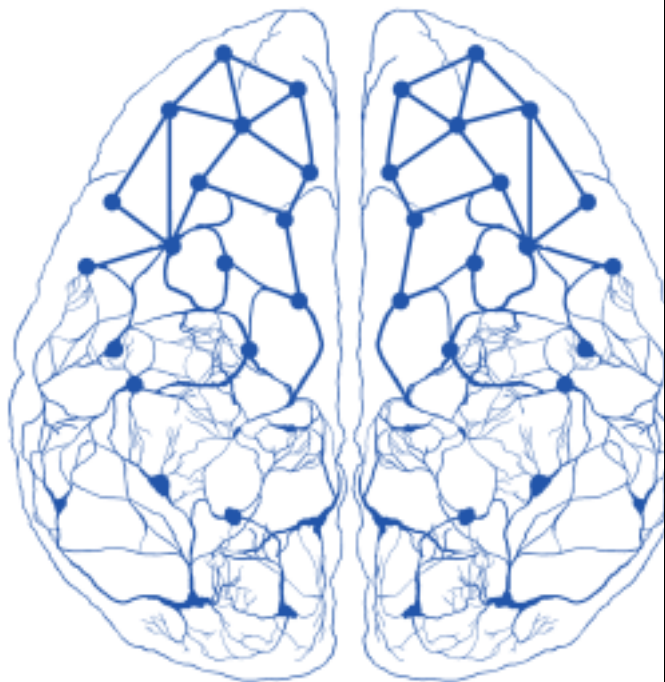
The project focused on automating the processing and updating of a Microsoft Access database used for medical data management. The goal was to replace the manual process with a reliable tool that significantly reduced the time needed for regular updates while also minimizing the risk of human error.

The result of the project is an application for automated processing of update data, accompanied by documentation for end users. The solution includes a mechanism for distributing new versions directly from GitLab, which facilitates future maintenance and deployment of further modifications.

	Client: prof. MUDr. Petra Lišková, M.D., PhD. Department of Paediatrics and Inherited Metabolic Disorders at 1st Faculty of Medicine CUNI
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In the works

	Deployment of JATOS and LimeSurvey on University Infrastructure For the needs of the Faculty of Arts, Charles University, we are preparing a proposal and validation of deploying research tools for online experiments and data collection (JATOS, LimeSurvey) on a unified infrastructure. The goal is to enable their reliable and long-term sustainable operation for the broader academic community. The work includes an analysis of existing deployments (VMs, load, data management), a proposal for containerization (Docker) and orchestration in Kubernetes, solutions for shared storage and external databases, and validation of scaling and operational limitations of the individual tools. Client: Mgr. Ondřej Tichý, Ph.D., Department of Linguistics at Faculty of Arts CUNI
	Thread Management Improvements for NBODY6/7 This project focuses on improving thread management in the NBODY6/7 simulation code to achieve more efficient use of computational resources. It also includes enhancements to the initialization of thread counts via program parameters and proper setup of thread affinity at startup. The goal is to ensure more stable and predictable performance for computationally intensive astrophysical simulations. Client: doc. RNDr. Ladislav Šubr, Ph.D. Astronomical Institute at Faculty of Mathematics and Physics CUNI
	Simulation-Based Calibration (SBC) for validating Bayesian models in Python The project's focus is the development of a modern Python implementation of the Simulation-Based Calibration (SBC) for validating Bayesian models. The goal is to create a modular and extensible architecture, which overcomes the limitations of current implementations, and enables an efficient work with various Bayesian frameworks, such as PyMC, Bambi or NumPyro. The implementation supports parallel processing of simulations, robust error handling, integration with the ArviZ library, and advanced diagnostic and visualization tools, including ECDF plots known from the reference implementation in the programming language R. The result is an open-source tool intended for research use as well as further development by the community surrounding Bayesian modeling. Client: Mgr. Martin Modrák PhD. Department of Bioinformatics at 2nd Faculty of Medicine CUNI

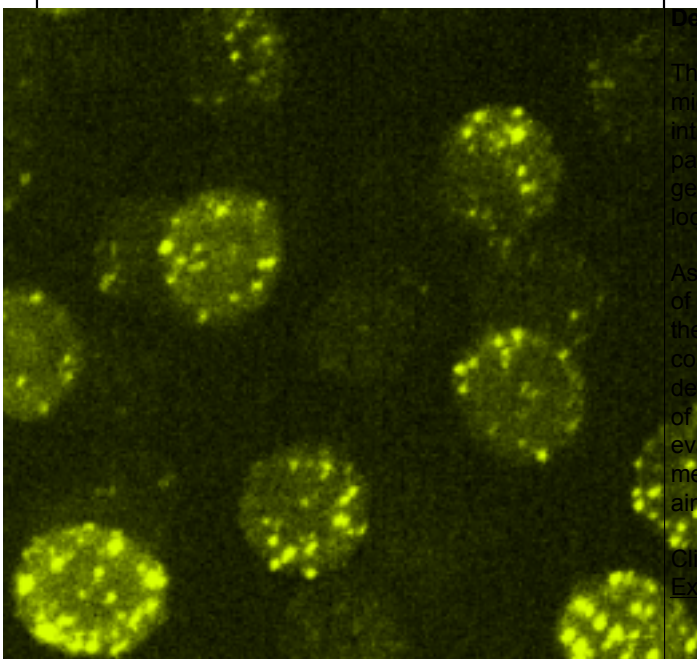


Optimization of MOZAIC for HPC in neuroscience

The project's focus is an analysis and optimization of the open-source framework MOZAIC used for simulation of biologically realistic neural networks. The goal is to identify performance limitations when running large-scale simulations on HPC infrastructure and to propose modifications leading to more efficient use of computing resources.

A part of the project is the deployment of a software solution comprising MOZAIC, NEST, and PyNN, as well as the profiling of real neuroscientific simulations and the analysis of their behaviour on various hardware platforms. Through collaboration with the framework's developers and users, we are exploring the possibilities of optimization of the configuration, compilation and the architecture of the application itself, the goal being a reduction of computation time and improvement of scalability in demanding HPC simulations.

Client: Mgr. Ján Antolík, Ph.D. Department of Software and Computer Science Education at Faculty of Mathematics and Physics CUNI



Detection of intracellular pathogens in plant cells

This project focuses on the automated processing of microscopic images of plant cells and the detection of intracellular structures associated with the presence of pathogens. The goal is to reliably identify individual cells, generate their masks and determine the amount and location of the observed point structures within each cell.

As part of this project, different approaches to processing of 2D and 3D image data are compared, including the analysis of individual microscopic sections and their composite representations. The solution includes the design of an effective pipeline of cell segmentation, pairing of the detected structures with specific cells, and an evaluation of the computational demand of each individual method. The project also utilizes GPU acceleration and aims to create a practical tool for use in biological research.

Client: Mgr. Adéla Příbylová, Ph.D. Department of Experimental Plant Biology at Faculty of Science CUNI