
Portfolio

Finished projects

	<p>Deployment of NEST Teaching Software on a Faculty HPC Cluster</p> <p>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.</p> <p>Client: Karolína Korvasová, M.Sc., Dr. rer. nat., Computational Systems Neuroscience Group MFF CUNI</p>
	<p>Running Origin Software on Linux for Scientific Data Analysis</p> <p>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.</p> <p>Client: doc. RNDr. Karel Carva, PhD., Department of Condensed Matter Physics MFF CUNI</p>
	<p>Containerization and Easy Installation of GBTOlib and UKRmol+</p> <p>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</p>



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 Kloperk'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 Kloperk, Ph D., [Department of Immunology, Second Faculty of Medicine, CUNI](#)



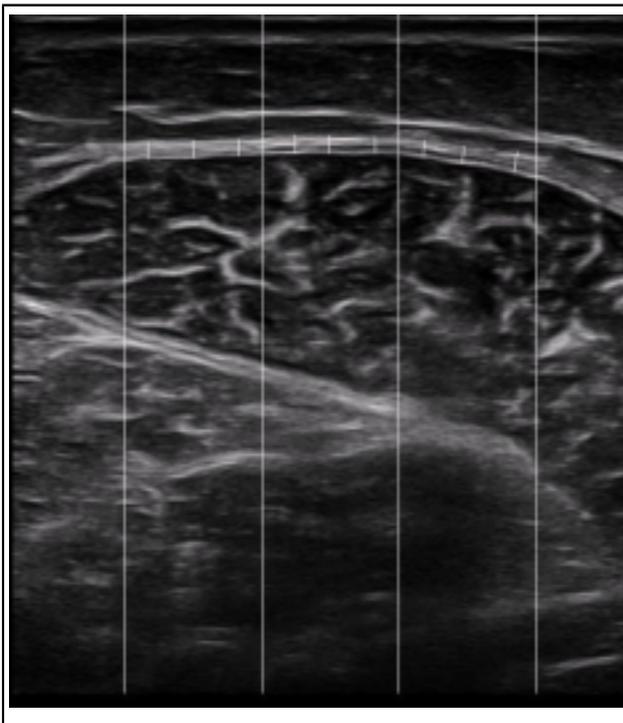
Web Interface for Risk Analysis (CLIP)

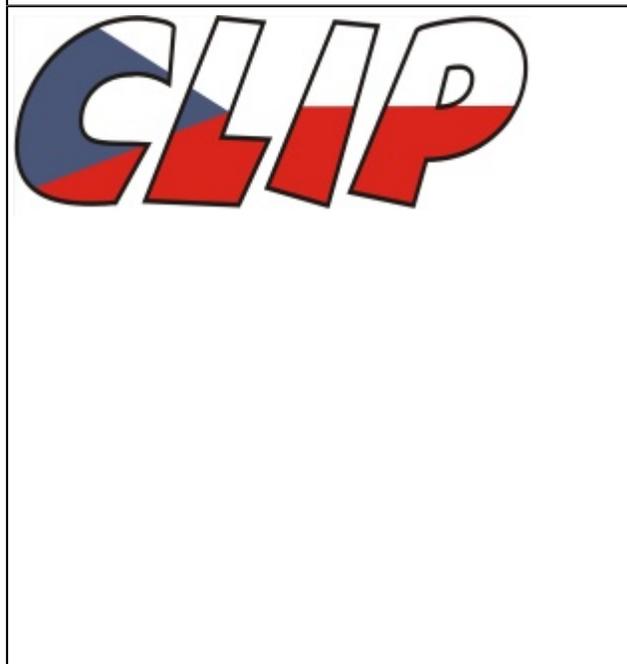
For the CLIP team, we created a simple web interface for monitoring risk development over time. Users upload evaluated risk tables (FMEA) for individual years (e.g., 2024, 2025, 2026) into the application, and the system automatically displays clear graphs showing changes in risk levels over the years.

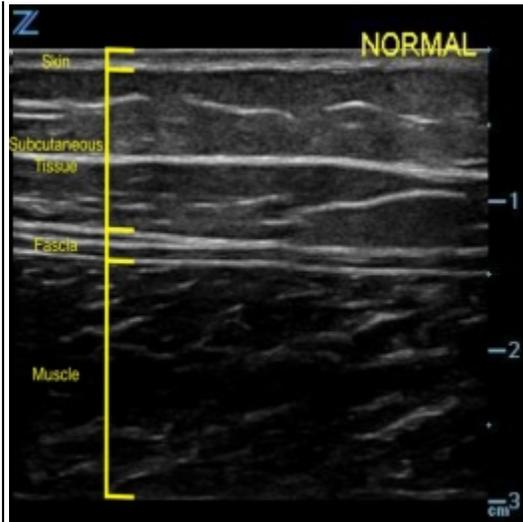
The goal was to replace manual work with spreadsheets and graphs and enable quick and clear evaluation of trends. The application is designed so that non-technical users can also use it, and it is available in Czech according to the client's requirements.

Client: Mgr. Jan Stuchlý, Ph.D., [Childhood Leukemia Investigation Prague \(CLIP\)](#)

Ongoing Projects

	<p>Automation of Deep Fascia Thickness Measurement from Sonographic Images</p> <p>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.</p> <p>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.</p> <p>Client: Mgr. Adéla Quittková, Department of Rehabilitation and Sports Medicine at Second Faculty of Medicine CUNI and Motol University Hospital</p>
	<p>Secure Deployment of Sensitive Cloud for Processing Sensitive Data</p> <p>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.</p> <p>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.</p> <p>Client: doc. JUDr. Jakub Drápal , M.Phil., Ph.D., <u>Faculty of Law, CUNI</u></p>
	<p>Web Platform for Vojta Method Study (SymBaby)</p> <p>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.</p> <p>We are preparing an application prototype with forms, user management, and change logging, including architecture design that allows physical data storage at Motol University</p>

	<p>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.</p> <p>Client: Mgr. Adéla Quittková, <u>Department of Rehabilitation and Sports Medicine at Second Faculty of Medicine CUNI and Motol University Hospital</u></p>
 <p>The logo features the word 'EVERSE' in purple, 'NETWORK' in a larger purple font, and 'RESEARCH SOFTWARE QUALITY' in a smaller, grey font below it. A blue line with circular nodes connects the text elements.</p>	<p>Project EVERSE – Research Software Quality and UDPipe</p> <p>As part of the European project <u>EVERSE</u> we contribute to the development and quality assessment of research software in the SSH (Social Sciences and Humanities) domain. Charles University's Faculty of Mathematics and Physics takes on the role of developer and maintainer of the UDPipe tool and actively participates in the implementation of quality principles defined within the project. Our activities connect the development of these tools with the EVERSE project.</p> <p>EVERSE builds an ecosystem of tools and methodologies, such as RSQKit (best practices and knowledge base), Research Software Quality Indicators (a set of quality indicators), QualityPipelines (automated evaluation of indicators), and Tech Radar (mapping of tools to quality domains). Our role is to assess and improve UDPipe according to these indicators, contribute experience from the SSHOC environment, and participate in connecting tools, training, and infrastructure solutions across the community.</p> <p>Client: Internal project</p>
 <p>The logo consists of the letters 'CLIP' in a bold, stylized font. The 'C' is blue and white, while the 'LIP' is red and white.</p>	<p>Implementation of WGS Pipeline into TSPS</p> <p>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> .</p> <p>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.</p> <p>Client: Mgr. Jan Stuchlý, Ph.D., <u>Childhood Leukemia Investigation Prague (CLIP)</u></p>
	<p>Autotracking of Aponeurosis Slip in Calf Muscle</p>



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