ELEGANCE: machinE LEarning for inteGrated multi-parAmetric eNzyme and bioproCess dEsign

DC 13: Development of ML-based tools for analysis and engineering protein dynamics

Organization

The Czech Technical University in Prague (CVUT) is one of the largest and oldest technical universities in Europe. The Czech Institute of Informatics, Robotics and Cybernetics (CIIRC) is a modern scientific institute of CVUT with nearly 300 employees working in eight research departments, complemented by specialized centers. CIIRC concentrates on cutting-edge fundamental and applied research in a variety of fields of computer science and artificial intelligence, focusing on four key areas: manufacturing, energy, smart cities, and a healthy society. CIIRC builds a unique ecosystem for artificial intelligence, interconnecting the industry, in particular SMEs, and universities in the Czech Republic with the main European research and innovation networks. CVUT hosts the ELLIS Unit Prague, which will provide the connection to the ELLIS network of machine learning researchers in Europe, the connection to the European ELLIS PhD program, as well as several European AI initiatives, including ELIAS (European Lighthouse of AI for Sustainability), ELLIOT (European Large Open Multi-Modal Foundation Models For Robust Generalization On Arbitrary Data Streams), and CLARA (Center for Artificial Intelligence and Quantum Computing in System Brain Research).

The doctoral candidate (DC) will work in the Intelligent Machine Perception group (IMPACT) led by Josef Sivic, a recipient of ERC Starting and ERC Advanced grants. The IMPACT team has expertise in developing new machine-learning methods and software for dynamic 2D and 3D data, including neural networks for molecular representations of proteins and their dynamics. The team's work was awarded several prizes, including the Helmholtz Prize and the Longuet-Higgins Prize, and won international competitions such as the 2020 and 2023 BOP challenge. The team develops machine-learning models to tackle real-world challenges in protein engineering and drug discovery. Key open scientific questions include: 1) Protein Dynamics & Interactions: How can we model and engineer protein dynamics (JACS Au, ICLR) and protein-protein interactions (ICLR)? 2) Enzyme Characterization: How to automatically characterize enzymes and predict outputs of enzymatic reactions (bioRxiv)? 3) Molecule Discovery: How to identify new molecules from mass spectrometry data in metabolomics (NeurIPS, Nature Biotechnology)? This research is conducted in collaboration with molecular biology experts, including Jiri Damborsky and his team at Loschmidt Laboratories, Masaryk University in Brno, and Tomas Pluskal from IOCB Prague. Breakthrough progress on these problems could lead to a deeper understanding of Alzheimer's disease mechanisms or the development of new drugs for acute stroke and other critical conditions.

Roles and responsibilities

We are looking for strongly motivated candidates with a background in machine learning or computational biology and an interest in AI for life sciences. The PhD will be carried out in 4 years at the Czech Technical University in Prague (CVUT, Czech Republic) under the supervision of Dr. Josef Sivic and Dr. Jiri Sedlar at the Czech Institute of Informatics, Robotics and Cybernetics (CIIRC). Within the first three years, an academic research stay (of 3 months) will take place at the Free University of Berlin (FUB, Germany) under the supervision of Prof. Dr. Cecilia Clementi. Additionally, an industrial

secondment (of 3 months) will take place at the company Novonesis (NVS, Denmark) under the supervision of Lars Olsen. We offer a competitive salary and work on cutting-edge research with high-impact applications. The aim is to publish in top-tier machine learning conferences, such as NeurIPS, ICLR, and ICML, or in high-impact biology journals (see the list of our publications). The position includes the opportunity (not a requirement) of participating in teaching and co-advising Bc/MSc students. The Horizon Europe Marie Sklodowska-Curie Actions (MSCA) Doctoral Network (DN) project starts in January 2026. The recruitment is planned for January to April 2026, with the start of the PhD project scheduled for May to October 2026. Your PhD degree will be awarded based on the successful completion of the research work at CVUT. You will also be required to participate in the training events organized by the DN. As an MSCA fellow, you are also expected to contribute to the dissemination of your PhD results via public engagement and other scientific platforms.

The PhD project will develop machine learning tools for predicting and engineering protein flexibility. Protein flexibility refers to the dynamic ability of protein structures to undergo conformational changes, which is fundamental to their biological function, enzymatic activity, and binding affinity. Predicting this flexibility computationally is crucial, as it enables the design of more stable and efficient enzymes for industrial and therapeutic applications without relying solely on expensive and time-consuming wet-lab experiments.

The PhD project will focus on:

- Development of advanced machine learning tools for the prediction of protein flexibility as a proxy for protein dynamics
- Acquisition of datasets by molecular dynamics (MD) simulations under different conditions (such as temperature)
- Development of advanced generative machine learning tools for the engineering of protein flexibility
- Fine-tuning of the tools and thorough validation on the case studies from project partners

Primary supervisors: Dr. Josef Sivic and Dr. Jiri Sedlar (CVUT)
Secondary supervisors: Prof. Dr. Cecilia Clementi (FUB), Lars Olsen (NVS)
Recruiting institution: Czech Technical University in Prague (CVUT)
Researcher profile: First Stage Researcher (R1)

Qualifications:

- MSc (or equivalent) in computer science, bioinformatics, biochemistry, or related area, preferably with experience in machine learning and artificial intelligence. Candidates with a bioinformatics or biochemistry background are welcome, but need to have the motivation to learn about machine learning and AI.
- Eligible as a graduate student at the Czech Technical University in Prague (CVUT)
- Research experience or interest in molecular biology and protein engineering
- Excellent communication skills for working within an interdisciplinary research team
- Strong analytical skills, high motivation, and ability to work independently
- Integrative and cooperative personality with excellent social skills
- Excellent English proficiency in written and oral form

Preferred (but not mandatory) qualifications:

- Experience with automation and coding in Python or other programming languages
- Experience with developing machine learning models
- Experience with protein software tools like AlphaFold3, Boltz2, PyMOL, etc.
- Interest in advanced machine learning and computational methods to improve and understand protein function
- Interest in entrepreneurship to make a positive impact on planetary and human health

Conditions of employment

You must hold a two-year master's degree (120 ECTS credits) or a similar degree with an academic level equivalent to a master's degree.

Approval and enrolment

The doctoral candidate will be enrolled in the Computer Science PhD program at the Faculty of Electrical Engineering at the Czech Technical University (CVUT).

We offer

We offer a rewarding job in an interdisciplinary international environment. We strive for academic excellence in an environment characterized by collegial respect and academic freedom. You will be part of an international team (IMPACT) based in a modern building in a nice neighbourhood of Prague, one of the most beautiful and expat-friendly cities in the world. The lab is located on the CVUT university campus, a 22-minute walk from the Prague Castle. You will have access to world-class infrastructure, including supercomputers Karolina and LUMI. Prague also has a vibrant AI scene. Work benefits include flexible working hours and occasional home office to support personal needs, six weeks of paid vacation per year, pension insurance contribution, a financial meal allowance, free language courses, an exclusive mobile tariff offer from Vodafone, and access to the Multisport card. The funding covers a living allowance (salary), a mobility allowance (private travel and accommodation), a family allowance (if applicable), a long-term leave allowance (if applicable), research, training, and networking events, as well as secondments.

Salary and appointment terms

The starting date is scheduled to be September 1st, 2026 (or October 1st, 2026, if necessary), but it is possible to start earlier, as mutually agreed upon. The doctoral candidate will be offered an employment contract, including social security coverage and health insurance, with a competitive remuneration based on the MSCA allowances in line with the MSCA WP 2023-2025. The income consists of a living allowance, mobility allowance, and, if eligible, family allowance. The total amount is EUR 4,483 - 5,143 (approximately CZK 108,700 - 124,700) per month, inclusive of all compulsory deductions, such as social security contributions, health insurance, and income tax. The position is full-time. The period of employment is 3 years, with possible extension supported by other research grant(s). You can read more about career paths at CVUT here.

Further information

Further information can be obtained from Dr. Jiri Sedlar (jiri.sedlar@cvut.cz) and Dr. Josef Sivic (josef.sivic@cvut.cz).
Website about the MSCA doctoral network ELEGANCE: https://elegance.dtu.dk
More information about CIIRC CVUT: https://www.ciirc.cvut.cz/en/
Intelligent Machine Perception (IMPACT) group: https://impact.ciirc.cvut.cz

Application procedure

Your complete online application must be submitted no later than January 31st, 2026 (23:59 Prague time). To be considered, the application must be submitted as a single PDF file containing all required materials.

To apply, please send your materials by email to jiri.sedlar@cvut.cz (cc josef.sivic@cvut.cz). Please attach all your materials in English to a single PDF file. The file must include:

- A letter of motivation (cover letter), including a statement of your research interests, relevant skills and experience, and an explanation for the choice of position
- Curriculum vitae, including a publication list (if applicable)
- Names and contact details of up to three referees willing to write confidential letters of recommendation
- Grade transcripts and BSc/MSc diplomas (in English), including an official description of the grading scale

You may apply prior to obtaining your master's degree, but you cannot begin before receiving it.

All interested candidates, irrespective of age, gender, disability, race, religion, or ethnic background, are encouraged to apply.

Selection process

Received applications will be considered carefully in line with the principles of the EU Charter and Code for Researchers. Selection criteria: (i) meeting qualification requirements described above, (ii) all required documents provided. Shortlisted candidates will be invited for a personal or online interview.