Simulations, Everyday Language, and AI in the Service of Future Anti-Cancer Medicine

Cancer diagnostics – especially during ongoing therapy – plays a crucial role in its effective treatment. Appropriately planned therapy not only reduces the risk of disease recurrence but also minimizes side effects, particularly in the case of tissue-sparing therapies aimed at preserving as much healthy tissue and organ function as possible. Therefore, the main goal of modern oncology is to predict how a tumor will develop after anti-cancer therapy and how best to tailor treatment to the individual patient's situation. Computational artificial intelligence methods are playing an increasingly important role in this process, allowing for the prediction of disease progression and responses to various treatment regimens. Unfortunately, precisely and quickly simulating complex biological processes still poses a serious challenge. This is one of the key bottlenecks in the development of so-called predictive medicine – which not only treats but also anticipates disease development and adjusts therapy in advance.

The project we are working on addresses this problem by creating a new generation of computational models for rapid tumor evolution modeling using artificial intelligence (AI). Our approach is based on hybrid methods – combining machine learning (data-driven models) with classical simulation based on biological knowledge and mathematical models. One of the key innovative elements will be the development of so-called encoder-processor-decoder generative architectures utilizing the latest models based on deep neural networks. These will enable the creation of models that can combine sparse clinical data with rich, artificially generated data from computer simulations. The result will be a system capable of predicting tumor development under various treatment options.

To enable wider application of such models – not only by computer scientists and systems biologists but also by clinicians – we will also introduce a natural language-based interface. For this, we will use modern large language models (LLMs) and the RAG (Retrieval-Augmented Generation) approach, which will combine knowledge from various fields: oncology, pharmacology, and computer modeling. The outcome of our project will be a novel system: Language-Driven Therapy Design (LDTD). This means therapy design assisted by natural language. Doctors and researchers will be able to use ordinary commands in colloquial language to create, analyze, and modify personalized forms of cancer treatment with the help of computer simulation.