Master thesis

To students at the Technical Faculty
(Medical Engineering / Medizintechnik, Computer Science/ Informatik / Artificial Intelligence, Data Science, LifeScience)

Title: Integrate AI with Mechanistic Modeling to Understand Cancer Growth and Resistance

Background: Head and neck cancers are the 6th most common cancer. Among anatomical subsites, laryngeal cancer is the most frequent type, accounting for 30 – 40% of cases. Representative models to evaluate chemotherapy agents remain a significant gap in head and neck cancer research. Computer simulation has been harnessed to capture key characteristics of the cancer and predict tumor response to chemotherapeutic agents.
Computational approaches, like those of agent-based models (ABM), have substantially accelerated research in oncology. ABM can be programmed to simulate individual cells' actions (e.g., migration, proliferation, death) and their collective, emergent behavior (e.g., metastasis). Spatial intratumor heterogeneity, e.g., cell phenotypes in hypoxic versus normoxic microregions, can also be precisely simulated at a single-cell resolution. However, for mechanistic models like ABM, a large number of unknown parameters have posed substantial costs on model accuracy and computing resources.
Current state: A preliminary ABM, implemented in *Netlogo*, of laryngeal cancer is developed in Prof. Li-Jessen's lab recently. Now, the model needs to be refined for its biological representation and computing efficiency.

Research questions: Which AI techniques and its deployment can improve ABM's fidelity and efficiency? What parameters and considerations are needed to improve results?

Methods & tasks:

1. Obtain a basic understanding of the biological assumptions underlying the current ABM.
2. Program additional agent-rules to enhance the biological representation of current ABM with support from another trainee from quantitative biology at McGill.
3. Survey current protocols of integrating AI into mechanistic biological model
4. Identify specific needs for the use of AI for this current ABM. Possible applications include: employing AI to derive agent-rules, developing AI surrogate models, employing ML for exploring relations between model parameters and employing ML to analyze ABM outputs.
5. Choose one application from the list above in discussion with the supervisors.
6. Perform simulation experiments to identify which AI techniques will support the proposed application.

Goal: Improve the fidelity and efficiency of an existing mechanistic model of laryngeal cancers with AI techniques.

The work will be supervised by **Prof. Dr.-Ing. Michael Döllinger** (Member of Department Informatics & AIBE)**.** The thesis is in **cooperation with Prof. Nicole Li-Jessen** (School of Communication Disorders, McGill University, Montreal, Canada)

We search for a dedicated and motivated student with

- experience in JAVA programming language (*Netlogo* is coded in JAVA)
- basic background in ABM based modeling
- a good knowledge in machine learning
- background in cell and molecular biology
- good written and verbal communication skills in English (cooperation partner is English speaking)

Contact persons:

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