

Bachelor Thesis/Research Project

Graphical User Interface (GUI) for Simulating Molecular Communication in Complex Vessel Networks

Background: In molecular communications (MC), information is conveyed using *signaling molecules*, e.g., between bio-chemical communication nodes. Within the human body, *natural* MC facilitates essential biological processes such as cellular signaling and neuronal communication. *Synthetic* MC builds upon these natural concepts to engineer MC systems, e.g., for medical applications, including early cancer detection [1], targeted drug delivery [2], and health monitoring [3].

MIGHT – A Model for MC in Vessel Networks (VNs): The human cardiovascular system (CVS) is envisioned as one of the premier application domains for in-body MC. Here, MC shall enable innovative medical applications and realize the vision of the Internet of Bio-Nano Things (IoBNT). At IDC, we have developed a mathematical model that captures the advection-diffusion-driven transport of signaling molecules within complex vessel networks, as found in the CVS. The model, named *Mixture of Inverse Gaussians for Hemodynamic Transport (MIGHT)*, predicts the spatiotemporal molecule concentration throughout the VN, due to the release of molecules at multiple points in the VN. As such, MIGHT can provide insights into the complex transport dynamics in large-scale VNs and aid the design of future MC applications in VNs. The model has been extensively validated via finite-element simulations [4] and a preprint has been published in [5].

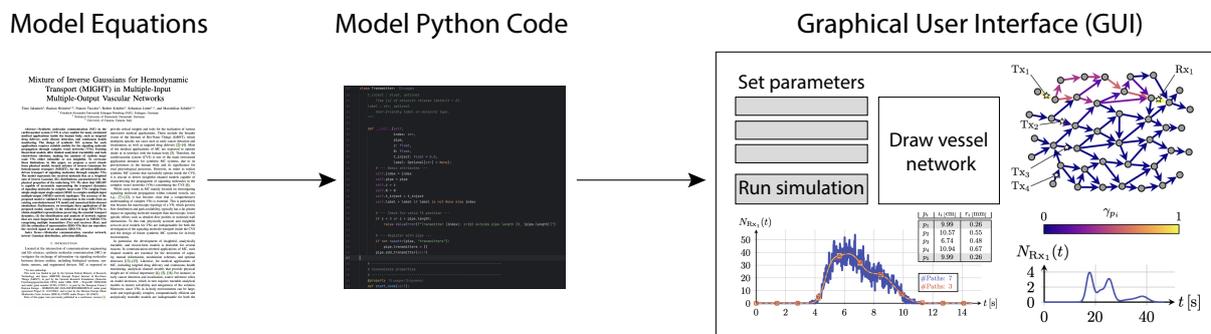


Figure 1: A GUI for creating VNs and simulating MC in VNs shall be developed in Python based on existing model code.

Overall Project Aim – Developing a GUI: To make the model more accessible to other researchers in the community, a GUI shall be developed that enables users to more easily simulate MC in VNs. The GUI will exploit existing object-oriented Python code for the simulation of the MIGHT model equations as its backend. The following functionalities should be included in the GUI: **1)** Users must be able to create VNs by placing nodes and edges in a graphical window, and by connecting them with vessels (i.e., edges). Parameter values such as vessel radii, inflow rates, number of released molecules, and hydraulic pressures at the VN outlets should be entered into appropriate fields in the GUI. Additionally, users should have the option to import/export VNs whose structure is stored in appropriate files (e.g., JSON). **2)** Once VNs have been created/imported and all required system parameters have been set, users should be able to run the model by pressing a button. Subsequently, received signals, e.g., in terms of

molecule concentration or flux, at desired points in the VN should be plotted as time-series. **3)** In [5], several exemplary applications of the model have been proposed. The GUI should offer the possibility to visually illustrate these applications for the created/imported VN. **4)** Finally, the GUI should be packaged into an executable file that is ready to run without the need for an integrated development environment (IDE) or the installment of any programming language.

Note that several of the envisioned tools for analysis and visualization have already been implemented individually. However, they have not been joined into a unified GUI.

Project Objectives: The main objectives of this thesis can be summarized as follows:

- Review and understand the MIGHT model in [5].
- Simplify and improve the structure of existing object-oriented Python code for the model.
- Create a GUI for the MIGHT model, including the following functionalities:
 - A window for drawing VNs by hand/loading VNs from memory/saving VNs to memory.
 - Buttons for simulating fluid flow and molecule transport in the VN, including color-coding of flow rates, molecule concentrations, and the plotting of received signals.
 - Plotting of selected model applications, including the structural reduction of VNs and the color-coding of the molecule transport importance of all vessels in the VN.
- Publication of the developed GUI, including the backend model code.

Prerequisites: The following qualifications are required in order to pursue this project:

- Basic understanding of mathematical modeling
- Advanced programming skills in Python

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References

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