Master thesis – *Masterarbeit*
for
Vorname Nachname
Student No.: XXXXXXXX

Thesis received: XX.XX.20XX	Workload: 720 h (24 CP)
Submission of thesis until: XX.XX.20XX	Duration: 6 months
First examiner: Prof. Dr.-Ing. U. Nackenhorst	Supervisor: Marlis Reiber
Second examiner: Prof. Dr.-Ing. Vorname Nachname	

Individual based Modelling of Quorum Sensing
Individuen basierte Modellierung von Quorum sensing

Biofilms are structured bacterial communities which are attached to a surface and are held together by self-produced extracellular polymeric substances (EPS) [2]. They can be beneficial in for example waste water treatment but can cause problems in the medical context where they cause infections in the host tissue or on implants. The formation of a biofilm consists of several steps and is influenced by many factors such as temperature, pH value, osmotic interactions, mixing and oxygen concentration [1]. Often smaller microcolonies consisting of several layers are formed and the bacteria start to multiply [3]. Bacterial cells can communicate via quorum sensing by releasing small diffusible molecules, the so-called autoinducers [6]. When a certain density is reached a synchronised change in the gene expression takes place facilitating the secretion of EPS [5]. The biofilm reaches a maximum growth where cell division and death are in equilibrium. Finally, the breakdown of the biofilm occurs, where bacteria detach and return into the planktonic state [1].

In addition to experiments, mathematical modelling of biofilms offers a deeper insight into the process of biofilm formation to prevent infections and efficiently use nonpathogenic biofilms.

Within the scope of this thesis a biofilm colonisation model using Individual based Modelling should be extended to include the process of Quorum sensing. For the simulation of the 3D dynamics of microbial communities the open-source IbM solver NUFEB[1] [4] which is an extension to the molecular dynamics code LAMMPS[2] should be used.

Required knowledge (to be covered in self-study where applicable): Basic programming skills are required, knowledge in C++ would be an advantage.

This thesis can be supervised/written in German or English language.

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[1]https://github.com/nufeb/NUFEB

[2]https://www.lammps.org/

The entire workload contains the following steps:

1. Preparing a milestone plan for a regular discussion of progress with the supervisor. The milestone plan needs to be handed in one week after receiving the task description. In case of circumstances, the milestone plan needs to be updated as agreed upon the supervisor. All versions of the milestone plan are to be submitted within the appendix of the thesis.

2. Literature review on biofilms in general and their modelling approaches in particular with special focus to the process of Quorum sensing

3. Familiarisation with LAMMPS and NUFEB and a brief description of its theoretical background and structure of code

4. Implementation of Quorum sensing. For that, the bacteria need to be able to sense the nutrient concentration around them, secrete autoinducers and start with the EPS production when a certain threshold is reached.

5. Systematic studies on the adjustment of model parameters based on in-vitro experiments described in literature

6. Documenting all steps and results regarding established scientific standards.

7. Self-evaluation of the own work using the attached evaluation matrix.

8. Creating a poster for the invitation to the presentation.

9. Presenting (15 to 20 minutes) the thesis within a colloquium.

In addition to an abstract in English and in German, five content describing key words have to be stated. The written report is to be submitted in one printed version. Additionally, all data are to be attached digitally.

Literature: *References

[1] S. Achinas, N. Charalampogiannis, and G. J. W. Euverink. A brief recap of microbial adhesion and biofilms. *Applied Sciences*, 9(14), 2019.

[2] J. W. Costerton, P. S. Stewart, and E. P. Greenberg. Bacterial biofilms: a common cause of persistent infections. *Science*, 284:1318–1322, 1999.

[3] H. Kanematsu and D. M. Barry. *Biofilm and Material Science*. Springer Berlin-Heidelberg, 2015.

[4] B. Li, D. Taniguchi, P. G. Jayathilake, V. Gogulancea, R. Gonzalez-Cabaleiro, J. Chen, A. S. McGough, I. D. Ofiter, T. P. Curtis, and P. Zuliani. Nufeb: A massively parallel simulator for individual-based modelling of microbial communities. *PLoS Computational Biology*, 15(12), 2019.

[5] M. B. Miller and B. L. Bassler. Quorum sensing in bacteria. *Annu Rev Microbiology*, 55:165–199, 2001.

[6] C. M. Waters and B. L. Bassler. Quorum sensing: Cell-to-cell communication in bacteria. *Annual Review of Cell and Developmental Biology*, 21:319–346, 2005.