Master Thesis Proposal

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1 Motivation

The motivation for the master thesis is the following model for the growth of marine biofilms:

$$\begin{cases} N_t = d_N \Delta N - \zeta N & \text{on } \Omega \times (0,T], \\ P_t = d_P \Delta P - \lambda P & \text{on } \Omega \times (0,T], \\ M_t = \delta \vec{\nabla}_\Gamma \cdot \left(D(M) \vec{\nabla}_\Gamma M \right) + f(C,N)M - h(M) - \lambda M & \text{on } \Gamma \times (0,T], \\ C_t = d_C \Delta_\Gamma C - \rho f(C,N) M - l(S) - \beta C & \text{on } \Gamma \times (0,T], \\ S_t = d_S \Delta_\Gamma S + \alpha M - \eta S & \text{on } \Gamma \times (0,T]. \end{cases} \tag{1.1}$$

Here, $\Omega \subset \mathbb{R}^3$ is some bounded Lipschitz domain with $\Gamma \subseteq \partial\Omega$. The tangential gradient, tangential divergence, and Laplace-Beltrami operator are defined respectively by

$$\begin{aligned} \vec{\nabla}_\Gamma u &:= \vec{\nabla} u - \frac{\partial u}{\partial \vec{\nu}} \vec{\nu}, \\ \vec{\nabla}_\Gamma \cdot \vec{F} &:= \vec{\nabla} \cdot \vec{F} - \frac{\partial \vec{F}}{\partial \vec{\nu}} \cdot \vec{\nu}, \\ \Delta_\Gamma u &:= \vec{\nabla}_\Gamma \cdot \vec{\nabla}_\Gamma u = \Delta u - \frac{\partial^2 u}{\partial \vec{\nu}^2}, \end{aligned}$$

where $\vec{\nu}$ denotes the unit outward normal vector to $\partial\Omega$. System (1.1) is supplemented with suitable initial conditions, and the boundary conditions

$$\begin{aligned} d_N \frac{\partial N}{\partial \vec{\nu}} &= -\mu f(C,N) M, & d_P \frac{\partial P}{\partial \vec{\nu}} &= h(M), & &\text{on } \Gamma; \\ \frac{\partial N}{\partial \vec{\nu}} &= 0, & \frac{\partial P}{\partial \vec{\nu}} &= 0, & &\text{on } \partial\Omega \setminus \Gamma; \end{aligned}$$

$$M = 0, \qquad \frac{\partial C}{\partial \vec{\nu}_\Gamma} = 0, \qquad \frac{\partial S}{\partial \vec{\nu}_\Gamma} = 0, \qquad \text{on } \partial\Gamma;$$

where $\vec{\nu}_\Gamma$ denotes the unit outward normal vector to $\partial\Gamma$.

The equations describe the development of a marine biofilm, that grows on (part of) the surface of some fluid-filled container, in dependence of several nutrients that affect its growth. The biofilm is so thin compared to the size of the container, that we may neglect its three-dimensional shape and instead model it as a cell density on the two-dimensional surface Γ.

The variable $M \in [0,1)$ denotes the normalised biomass density of the biofilm, with $M = 0$

meaning no cells present and $M = 1$ being the maximum possible saturation. The region $\{\vec{x} \in \Gamma \mid M(\vec{x}, t) > 0\}$ represents the actual biofilm at time t. The diffusion operator $D(M)$ has a singularity at $M = 0$, which ensures that the biofilm spreads at a finite speed with a sharp front; and a degeneracy at $M = 1$, which ensures that the biomass density remains bounded by some constant strictly less than 1. The variables N, P, C, and S denote the concentrations of dissolved nitrogen, free-floating planktonic cells, dissolved carbon, and carbon solubilisation factors respectively. The biofilm grows through the uptake of dissolved nitrogen and carbon, represented by the function f. The carbon is initially part of the solid substrate Γ and cannot be used directly by the biofilm cells. The cells produce a special solubilisation enzyme at a constant rate α, that dissolves the carbon, freeing it from the substrate permanently (described by the function l). Both the solubilisation factor and the dissolved carbon are assumed to largely stay within the biofilm, so we only consider their concentrations on Γ. Cells occasionally detach from the biofilm and enter the liquid bulk Ω, where they remain. The concentration of these planktonic cells is modelled by the variable P, and the detachment process by the function h.

2 Goals and challenges

The thesis will focus on the numerical analysis and simulation of the model. The finite element method lends itself well to systems of parabolic equations such as (1.1), hence it will be used to discretise in space. For the time discretisation, a semi-implicit method will be used that was developed in [3] for simpler systems in bounded domains. This method has the benefit of decoupling the equations, while maintaining the favourable stability properties of a fully implicit method. In [3], the author also deals with the degenerate and singular diffusion operator D, which has to be regularised in order for the numerical method to behave nicely.

The main new difficulty of (1.1) lies in the bulk-surface coupling. This makes both the analytical and numerical analysis significantly more involved. The potential for the surface Γ to be curved complicates the analysis even further.

The software FreeFEM++[1] is used to facilitate solving the variational problem that arises after time discretisation when writing (1.1) in the weak form. It allows us to focus on the behaviour of the model and the numerical approximation, without having to go through the arduous process of implementing the finite element method ourselves.

Depending on feasibility and time constraints, we may also explore error estimation for a simplified version of the model with a flat surface Γ. A posteriori estimates are of particular interest, as they can be used for adaptive meshing (which is appealing since we expect $\vec{\nabla}_\Gamma M$ to be highly variable in space). However, a priori estimates for singularly degenerate diffusion problems have been derived before[2] and may be more suitable for this thesis. Introducing cell reattachment to the model would be interesting to explore, but likely beyond the scope of this thesis.

Bibliography

[1] F. Hecht. "New development in FreeFem++". In: *J. Numer. Math.* 20.3-4 (2012), pp. 251–265. ISSN: 1570-2820. URL: `https://freefem.org/`.

[2] Florin Radu, Iuliu Pop, and Peter Knabner. "Error estimates for a mixed finite element discretization of some degenerate parabolic equations". In: *Numerische Mathematik* 109 (Jan. 2007), pp. 285–311. DOI: `10.1007/s00211-008-0139-9`.

[3] R. K. H. Smeets et al. *Robust time-discretisation and linearisation schemes for singular and degenerate evolution systems modelling biofilm growth*. 2024. arXiv: `2404.00391 [math.NA]`. URL: `https://arxiv.org/abs/2404.00391`.