Numerical Computations of a Multiphase System for Biofilm Development

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Motivation

Bacterial biofilms:

- affect numerous environmental, medical, and industrial processes
- are more resistant to antimicrobial agents than are planktonic cells
- persistence is likely due to a combination of phenotypic, environmental, and structural mechanisms

Theoretical Approach

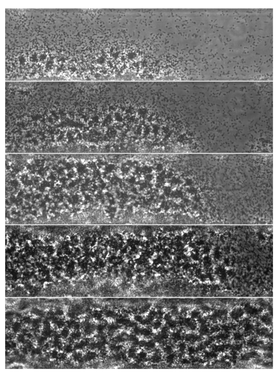
We formulate a mathematical model using a multiphase framework to capture these varying mechanisms of biofilm development.

The Big Question

In absence of analytical solutions, how can we efficiently and reliably simulate the dynamics of this nonlinear system of coupled PDEs?

Experimental Insight

- De La Fuente, et al., at Auburn University have engineered microfluidic channels to experimentally reproduce biofilm formation in the xylem of grape vines [2]
- observed spatial patterning is used to estimate parameters through perturbation analysis of the unstable modes of the linearized system



Multiphase Framework

$\phi_b \rightarrow$ free bacteria (unbound)
$\phi_{nb} \rightarrow$ network bacteria (bound)
$\phi_{eps} \rightarrow$ extracellular polymeric substance (EPS)
$\phi_f \rightarrow$ fluid

- network bacteria and EPS are stationary
- free bacteria move with the fluid
- network bacteria become unbound with rate a_1
- free bacteria become bound with rate a_2
- bacteria grow to a threshold
- network bacteria produces EPS with rate c_1
- EPS degrades at rate c_2

$$\frac{\partial \phi_b}{\partial t} + \frac{\partial(\phi_b u_f)}{\partial x} = a_1(\alpha - \phi_{eps})\phi_{nb} - a_2\phi_b + D_b\frac{\partial^2 \phi_b}{\partial x^2} + r_b\phi_b(K_b - \phi_b)$$

$$\frac{\partial \phi_{nb}}{\partial t} = -a_1(\alpha - \phi_{eps})\phi_{nb} + a_2\phi_b + D_{nb}\frac{\partial^2 \phi_{nb}}{\partial x^2} + r_{nb}\phi_{nb}(K_{nb} - \phi_{nb})$$

$$\frac{\partial \phi_{eps}}{\partial t} = c_1\phi_{nb} - c_2\phi_{eps} + D_{eps}\frac{\partial^2 \phi_{eps}}{\partial x^2}$$

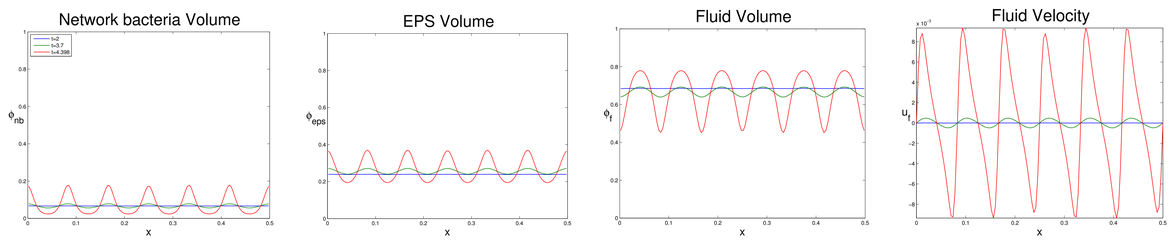
$$\frac{\partial \phi_f}{\partial t} + \frac{\partial(\phi_f u_f)}{\partial x} = -D_b\frac{\partial^2 \phi_b}{\partial x^2} - D_{nb}\frac{\partial^2 \phi_{nb}}{\partial x^2} - D_{eps}\frac{\partial^2 \phi_{eps}}{\partial x^2} - r_b\phi_b(K_b - \phi_b)$$
$$- r_{nb}\phi_{nb}(K_{nb} - \phi_{nb}) - c_1\phi_{nb} + c_2\phi_{eps}$$

$$\mu\frac{\partial}{\partial x}\left(2\phi_f\frac{\partial u_f}{\partial x}\right) - \phi_f\frac{\partial P}{\partial x} - \kappa_{fn}\phi_f\phi_{nb}u_f = 0$$

$$\nabla \cdot (\phi_f u_f + \phi_b u_f) = 0$$

$$\phi_b + \phi_{nb} + \phi_{eps} + \phi_f = 1$$

Numerical Computations



Scheme

- based on Wright, Guy, Fogelson [1]
- multigrid both as a standalone solver and as a right preconditioner for GMRES
- marker-and-cell (MAC) grid
- second-order finite differences
- explicit upwinding, implicit Euler
- periodic boundary conditions

Multigrid

- grid coarsening: restrict to 1 cell center
- transfer operators
  - restriction: full weighting for velocities, averaging for pressure/mass
  - prolongation: linear interpolation
- smoother: red-black box relaxation
- V- or F-cycling
- simulations in 1D

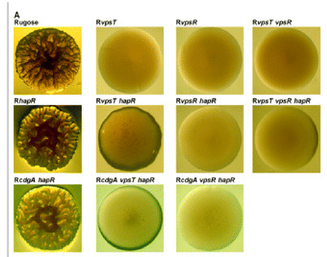
Conclusions

- successfully implemented an efficient and robust numerical scheme
- the dynamics of the system agree with the experimental biology
- extension to 2D, 3D

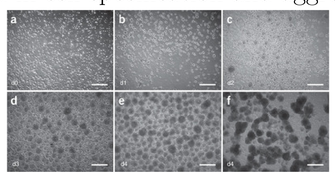
Future Work

This numerical scheme can also be applied to a variety of other problems, including

- rugosity - switch between smooth and rugose is linked to virulence factors and interplay between two EPS gene networks



- stem cell differentiation/proliferation - both mechanical and biochemical influences have been implicated in cell specification and aggregation



References

[1] G. B. Wright, R. D. Guy, A. L. Fogelson, SIAM J. Sci. Comput., **30** 2535-2565 (2008).

[2] Zaini, P.A., De La Fuente, L., Hoch, H.C., Burr T.J. FEMS Microbiology Letters, **295** 129-134 (2009).

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