Computational Aspects of Growth-Induced Instabilities with Applications to Biofilms

Berkin Dortdivanlioglu, Ali Javili & Christian Linder

Introduction

Biofilms, similar to other living materials, have the ability to grow and adapt in favor of their surroundings. The growth of biofilms is often due to the secretion of extracellular polymeric substances (EPS) produced by micro-organisms. Biofilm growth can form wrinkling or other more complicated folding patterns, overall referred to as growth-induced instabilities, depending on the specific geometry and the boundary conditions of the problem.

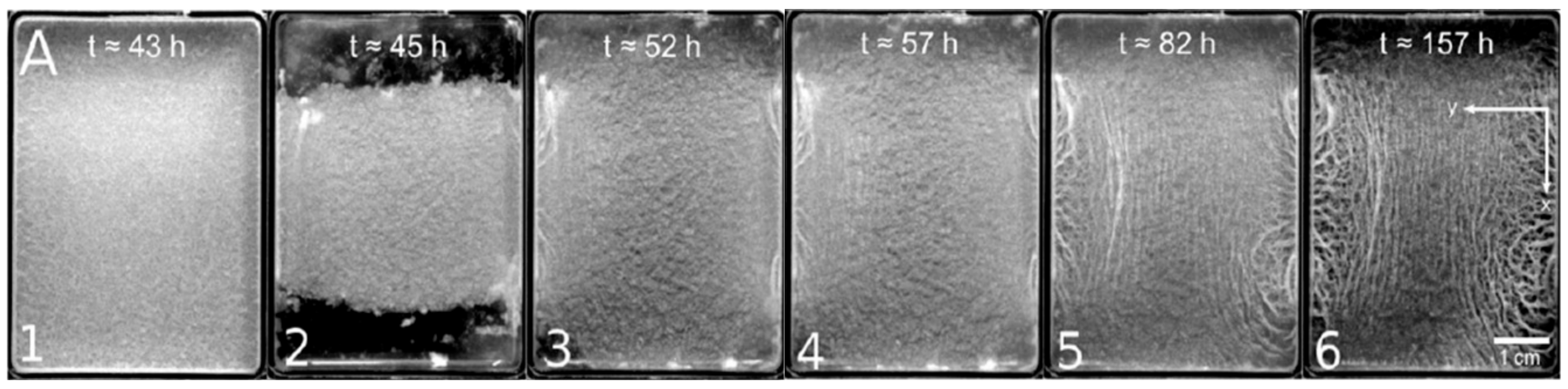


Figure: Experimental results [2] of biofilm structure evolving over time.

To successfully describe wrinkling phenomena at biofilms, we will:

- *establish* a computational framework to study growth-induced instabilities,
- *demonstrate* the robustness and accuracy of the established framework in a broad concept,
- *identify* key parameters on characteristic wavelength and growth of biofilm.

Computational model

Theory of Growth at Finite Strain

The continuum-based computational concept is used for the finite growth model. The growth is described by the multiplicative decomposition of the deformation gradient $\mathbf{F}$ into an elastic part, $\mathbf{F}^e$, and a growth part, $\mathbf{F}^g$:

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^g = \nabla\varphi \text{ where } \mathbf{F}^g = (1+g)\mathbf{I} \qquad (g\text{: growth parameter})\,.$$

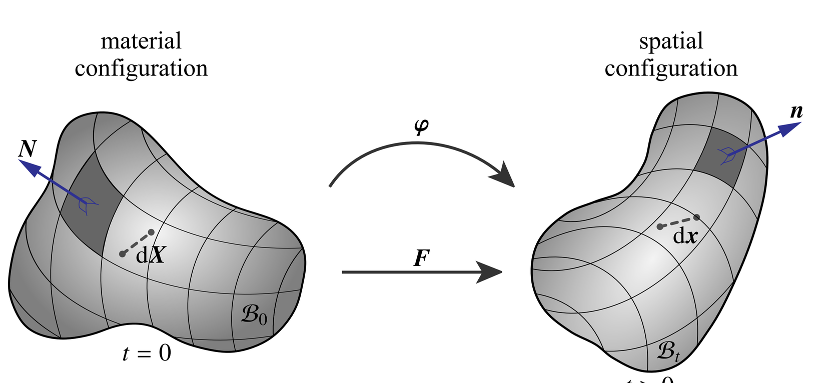


Figure: Kinematics in material & spatial configuration

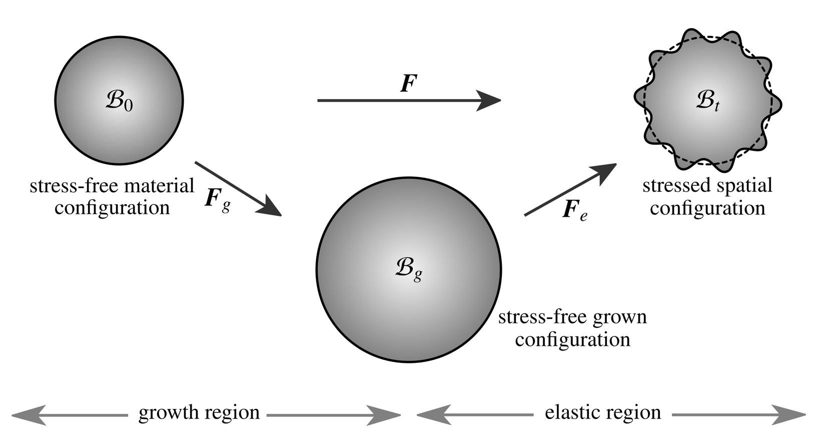


Figure: Kinematics of growth

Growth-Induced Instability

As the body $\mathcal{B}_0$ grows, stresses inside the body are induced due to the confinement. At a critical growth value (g_c), geometric instabilities are initiated in the form of wrinkling or folding.

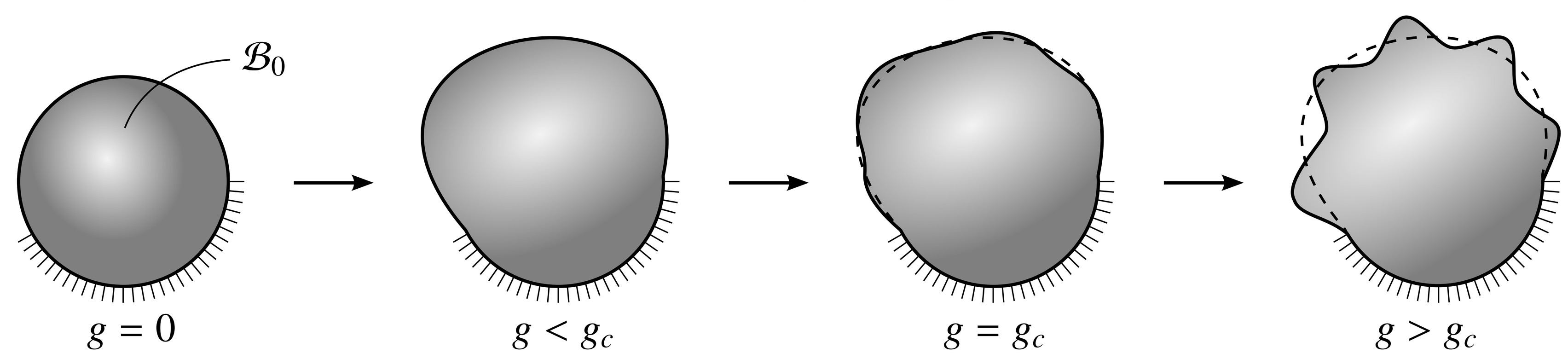


Figure: Formation of growth induced instability as growth parameter, g, increases.

The *finite element method* requires the solution of the following nonlinear system, e.i. the vanishing residual vector;

$$\boldsymbol{R}(\varphi) \stackrel{!}{=} \mathbf{0}\,.$$

Making use of Newton-Raphson scheme to solve above equation for φ, we linearize the resulting system of equations as;

$$\boldsymbol{R}(\varphi_{k+1}) = \boldsymbol{R}(\varphi_k) + \frac{\partial \boldsymbol{R}}{\partial \varphi}\Big|_k \cdot \Delta\varphi \stackrel{!}{=} \mathbf{0} \quad \text{and} \quad \varphi_{k+1} = \varphi_k + \Delta\varphi\,.$$

The stiffness matrix $\boldsymbol{K} := \frac{\partial \boldsymbol{R}}{\partial \varphi}\Big|_k$ and its eigenspace representation is $\boldsymbol{K} = \sum_{i=1}^{n} K_i \boldsymbol{\lambda}_i \otimes \boldsymbol{\lambda}_i$.

By the symmetry of $\boldsymbol{K}$ and the orthogonality property of eigenvectors, we have;

$$K_i \Delta\varphi_i = R_i \qquad \forall i \in \{1,..,n\} \qquad \text{(no sum)}\,.$$

Eigenvalue Analysis vs Perturbation Method

We demonstrate a more accurate and robust approach using *eigenvalue analysis* to capture the growth-induced instabilities compared to the common approach *perturbation method*. Using Eigenvalue analysis and without prescribing any perturbation to the system, we keep track of the smallest eigenvalue as it goes towards zero. At The time it becomes zero we obtain the instability mode.

Three Representative Examples

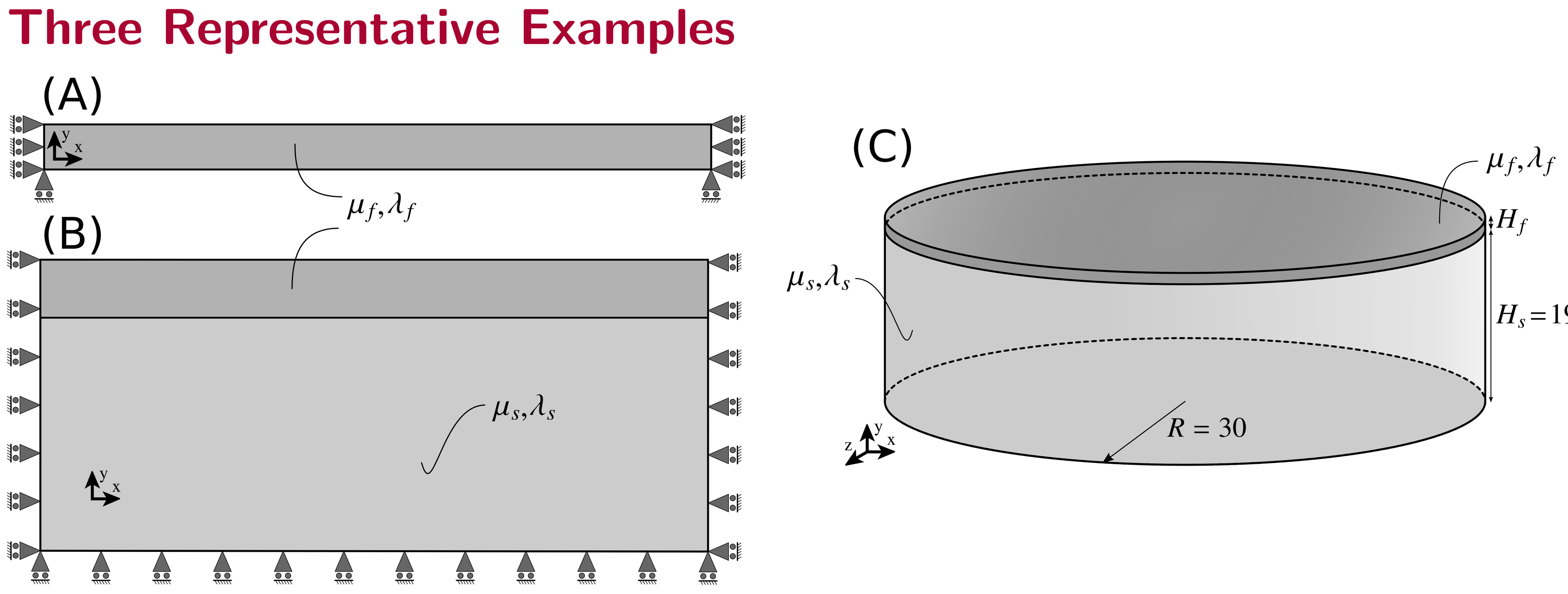


Figure: (A) Bifurcation study of a growing slender beam, (B) Instability study of a growing film on a soft substrate, (C) 3D instability study of a growing film on a soft substrate.

Results

Bifurcation Study of a Growing Slender Beam

Analytical solution:

$$w(x) = \frac{1-\cos\alpha}{\sin\alpha - \alpha}\left[\sin\left(\alpha\frac{x}{L}\right) - \left(\alpha\frac{x}{L}\right)\right] + \cos\left(\alpha\frac{x}{L}\right) - 1 \quad \text{where} \quad \alpha = 2\frac{L}{H}\sqrt{3g}\,.$$

For each mode, the following deformations are obtained;

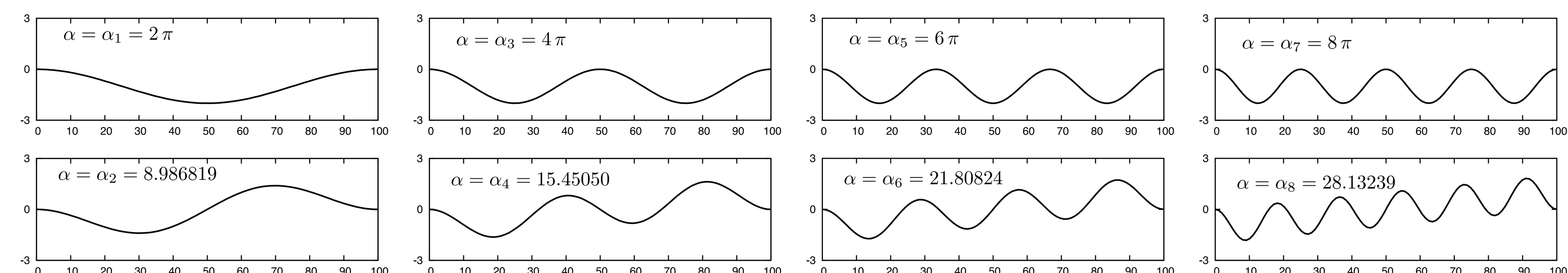
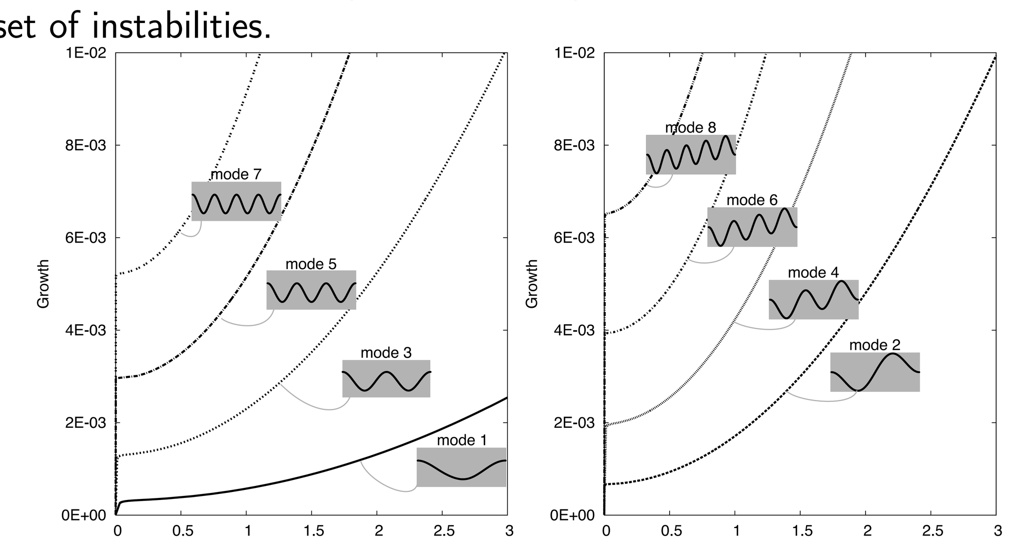


Figure: The critical growth g_c corresponds to $\alpha_i's$ where $i = 1^{st}, 2^{nd}, ..., 8^{th}$ mode.

Numerical investigation by eigenvalue analysis: We **explore the influence** of different finite element types and mesh quality, and compare the results to analytical solutions. We observed that, for example, 12 quadratic elements (142 DOFs) are much more accurate than 48000 linear elements (107998 DOFs) when $\nu = 0.49$. Moreover, eigenvalue analysis accurately captures the onset of instabilities.

Bifurcation tree by perturbation: Insight obtained enables us to compute the complete bifurcation tree. Perturbations are chosen as small as possible.



Instability study of a growing film on a soft substrate

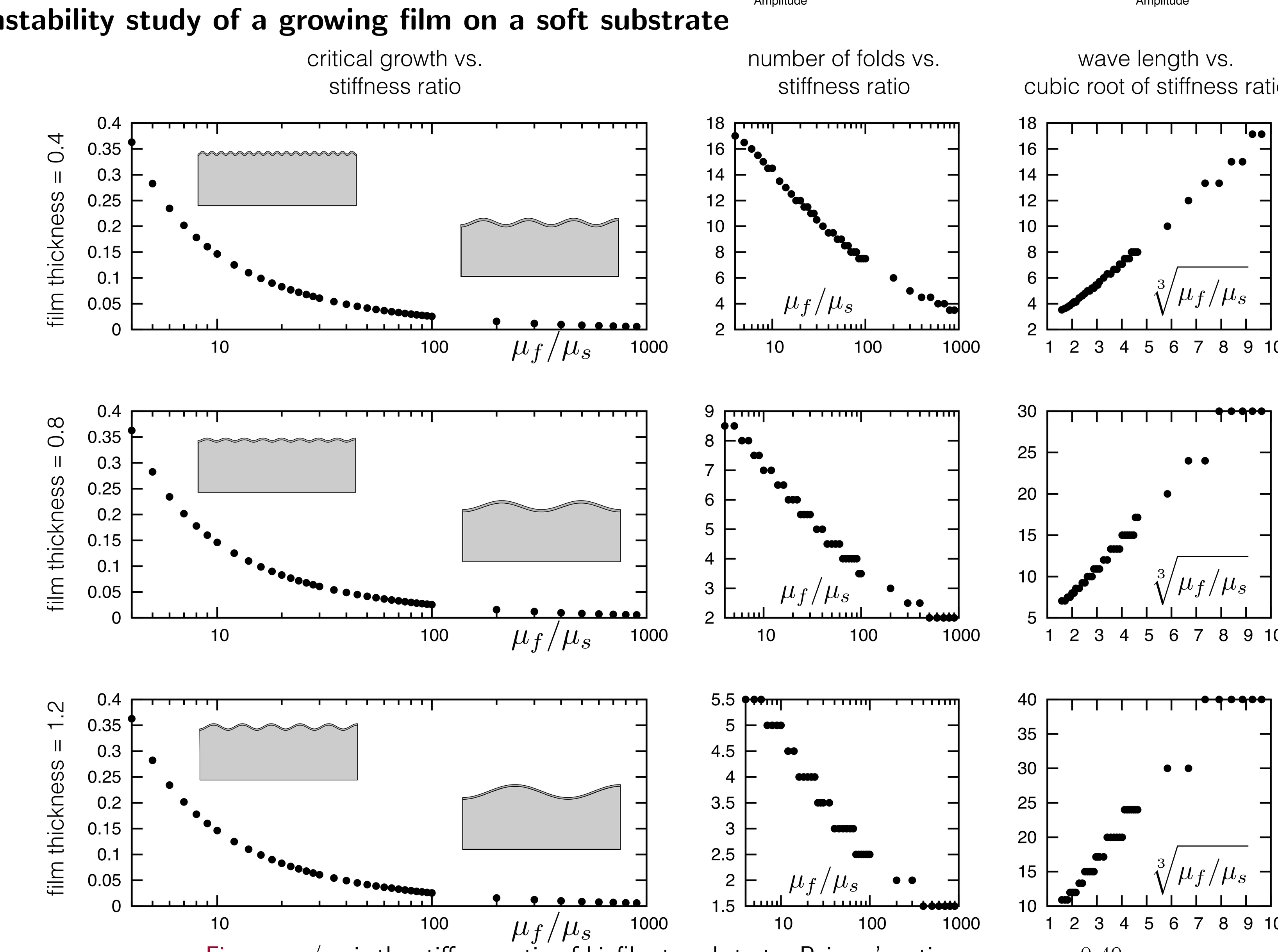
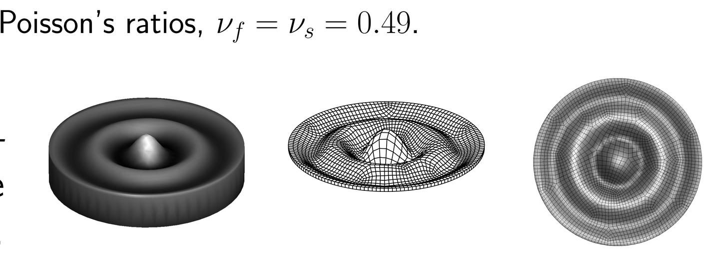


Figure: μ_f/μ_s is the stiffness ratio of biofilm to substrate. Poisson's ratios, $\nu_f = \nu_s = 0.49$.

3D instability study Eigenvalue analysis is *perturbation-free* and *independent of time step*. We require roughly 20 iterations to compute critical growth with 4 digits of accuracy. To achieve same accuracy, perturbation method requires at least 10^4 iterations.



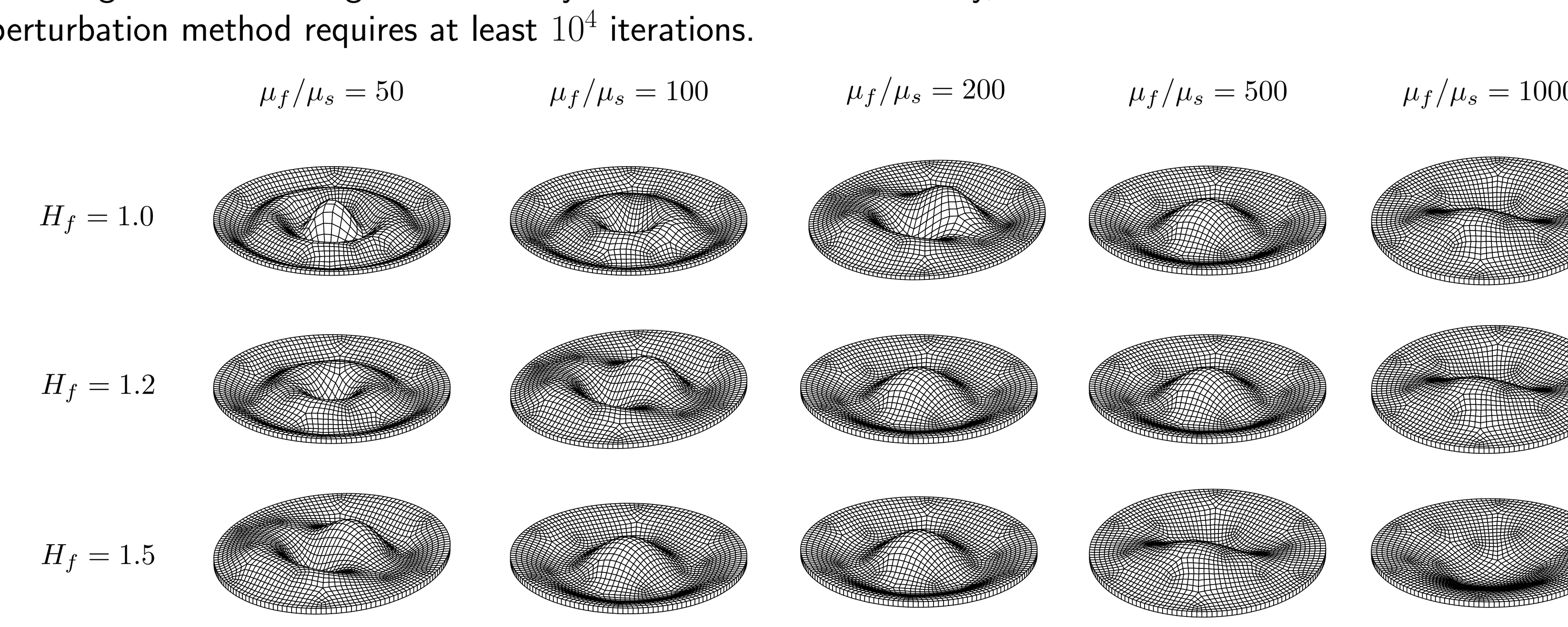


Figure: Instability behavior for different thicknesses and stiffness ratios. The substrate is removed for clarity.

Future goals

Further investigation of performances of mixed and enhanced finite element types. Propose a new class of enhanced finite element suitable for growth and growth-induced instabilities. Detailed study of period-doubling and -tripling phenomena observed in bilayer systems.

References

[1] E. Kuhl, A. Menzel & P. Steinmann (2003). *Comput. Mech.* 32:71-88.
[2] M. Trejo et al. (2013). *Proc. Nat. Acad. Sci* 110:2011.
[3] A. Javili et al. (2015). *Comput. Mech.* 56(3):405-420.
[4] B. Dortdivanlioglu, A. Javili & C. Linder (2017). *Comput. Methods Appl. Mech. Eng.* 316:261-279.
[5] B. Dortdivanlioglu & C. Linder (2019). *J. Mech. Phys. Solids* 125:38-52.

Stanford | ENGINEERING
Civil & Environmental Engineering
Stanford University
Stanford | DOERR
School of Sustainability