Biofilm FEM Stress Pipeline

From TMCMC Parameter Estimation to 3D Abaqus Stress Analysis

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1 Overview

This report documents the complete finite-element mechanical analysis pipeline built on top of the 5-species Hamilton biofilm model. TMCMC parameter estimation (in `data_5species/`) yields posterior samples $\theta \in \mathbb{R}^{20}$, which drive a 3D reaction–diffusion FEM simulation of species volume fractions $\varphi_i(\mathbf{x})$. The resulting dysbiotic index field $\mathrm{DI}(\mathbf{x})$ is then used to drive a spatially heterogeneous elastic modulus field, which is finally solved in Abaqus for stress.

Pipeline Summary

Stage	Script	Output
TMCMC estimation	`estimate_reduced_nishioka.py`	θ_{MAP}, posterior samples
FEM species field	`fem_3d_extension.py`	$\varphi_i(\mathbf{x})$, 15^3 grid
Posterior ensemble	`run_posterior_abaqus_ensemble.py`	20 samples $\times$ 4 conditions
B1: DI credible interval	`aggregate_di_credible.py`	p05/p50/p95 DI fields
A: Material sensitivity	`run_material_sensitivity_sweep.py`	$E_{\mathrm{max},E_{\mathrm{min},n}}$ sweep
C1: Anisotropy gradient	`fem_aniso_analysis.py`	$\nabla\varphi_{Pg}$, dominant $\mathbf{e}_1$
C1: Aniso Abaqus sweep	`run_aniso_comparison.py`	$\beta \in \{1.0, 0.7, 0.5, 0.3\}$
B3: CZM interface	`run_czm3d_sweep.py`	R_F^{peak}, G_c^{eff}

2 Physics

2.1 Dysbiotic Index

The dysbiotic index is computed from the Shannon entropy of the 5-species composition:

$$H(\mathbf{x}) = -\sum_{i=1}^{5} \frac{\varphi_i}{\Phi} \ln\left(\frac{\varphi_i}{\Phi}\right), \qquad \Phi = \sum_{i=1}^{5} \varphi_i \tag{1}$$

$$\mathrm{DI}(\mathbf{x}) = 1 - \frac{H(\mathbf{x})}{\ln 5} \quad \in [0, 1] \tag{2}$$

where DI = 0 corresponds to a perfectly commensal (uniform) composition and DI = 1 corresponds to complete dysbiosis (single-species domination).

2.2 E(DI) Power-Law Mapping

The elastic modulus varies with the local dysbiotic index via a power law:

$$r(\mathbf{x}) = \min\left(1,\ \max\left(0,\ \frac{\mathrm{DI}(\mathbf{x})}{s}\right)\right), \qquad s = 0.025778 \tag{3}$$

$$\boxed{E(\mathbf{x}) = E_{\mathrm{max}(1-r)^n + E_{\mathrm{min}}\, r}} \qquad E_{\mathrm{max}=10\text{ GPa},} \quad E_{\mathrm{min}=0.5\text{ GPa},} \quad {}_{n=2} \tag{4}$$

2.3 Transversely Isotropic Material (C1)

Motivated by the dominant gradient direction of *P. gingivalis* concentration $\nabla\varphi_{Pg}$, a transversely isotropic model is considered with stiff axis $\mathbf{e}_1$ aligned to $\nabla\varphi_{Pg}$:

$$E_1 = E(\mathrm{DI}), \qquad E_2 = E_3 = \beta \cdot E_1, \qquad \beta \in [0, 1] \tag{5}$$

$$\nu_{12} = \nu_{13} = \nu_{23} = \nu = 0.30, \quad G_{12} = G_{13} = \frac{E_1}{2(1+\nu)}, \quad G_{23} = \frac{E_2}{2(1+\nu)} \tag{6}$$

This is implemented in Abaqus via `*ELASTIC, TYPE=ENGINEERING CONSTANTS`. The orientation is defined by a datum coordinate system aligned to $\mathbf{e}_1$ computed from the median $P.g$ gradient field, and applied globally via `part.MaterialOrientation(orientationType=SYSTEM, axis=AXIS_1)`.

2.4 Cohesive Zone Model (B3)

The biofilm–substrate interface is modelled as a zero-thickness cohesive layer with DI-dependent cohesive properties:

$$t_{\max(\mathrm{DI})=t_{\max,0}(1-r)^n}, \qquad G_c(\mathrm{DI})=G_{c,0}(1-r)^n \tag{7}$$

with $t_{\max,0} = 1.0$ MPa and $G_{c,0} = 10.0$ J/m^2. Mixed-mode damage evolution follows the Benzeggagh–Kenane (BK) criterion.

3 Conditions and Parameters

Table 1: 4 simulation conditions

Key	Label	a_{35} (Veillonella→Pg)	Description
`dh_baseline`	dh-baseline	21.4	Original dh TMCMC run
`commensal_static`	Comm. Static	3.56	Mild-weight θ, no HOBIC
`commensal_hobic`	Comm. HOBIC	3.56	Mild-weight θ + HOBIC
`dysbiotic_static`	Dysb. Static	20.9	No-lambda θ

Table 2: Key global parameters

Parameter	Value	Description
s (DI_SCALE)	0.025778	Global DI normalization
$E_{\max}$	10.0 GPa	Commensal stiffness
$E_{\min}$	0.5 GPa	Dysbiotic stiffness
n	2	Power-law exponent
ν	0.30	Poisson's ratio
N_{bins}	20	Material assignment bins
Grid	$15^3 = 3375$ nodes	FEM spatial resolution
Applied load	1.0 MPa	Compressive surface pressure

4 Results

4.1 A. Material Sensitivity Sweep

4.1.1 A1 – $E_{\max \times E_{\min}}$ Grid

A 4×4 parameter sweep over $E_{\max \in \{5,10,15,20\}}$ GPa and $E_{\min \in \{0.1,0.5,1.0,2.0\}}$ GPa (fixed $n = 2$, $\theta =$ dh_old) showed approximately linear scaling of S_{Mises} with $E_{\max}$, with $E_{\min}$ having secondary influence.

4.1.2 A2 – Power-Law Exponent

For $n \in \{1, 2, 3\}$: increasing n sharpens the transition at the substrate, producing higher peak stresses near DI-transition zones.

4.1.3 A3 – θ Variant Comparison

Table 3: A3: S_Mises at substrate for 3 θ variants

Variant	a_{35}	S_{Mises} sub.	S_{Mises} surf.	Δ sub.
mild_weight	3.56	–	–	$\approx -30\%$ vs dh_old
dh_old	21.4	reference	reference	–
nolambda	20.9	$\approx$ dh_old	$\approx$ dh_old	$< 5\%$

Key finding: *mild_weight* TMCMC result (Pg suppressed, $a_{35} = 3.56$) gives $\approx 30\%$ lower substrate stress than the unconstrained *dh_old* ($a_{35} = 21.4$), providing mechanical evidence that TMCMC regularization toward commensal biofilm is physically meaningful.

4.2 B1. DI Credible Interval

Table 4: B1: Posterior DI spread and substrate S_Mises (p50)

Condition	$\overline{\text{DI}}$ (p50)	$S^{\text{sub}}_{\text{Mises}}$ (MPa)
dh-baseline	≈ 0.015	≈ 0.84
Comm. Static	≈ 0.010	≈ 0.86
Comm. HOBIC	≈ 0.010	≈ 0.85
Dysb. Static	≈ 0.011	≈ 0.86

The p05–p95 stress band reflects biological uncertainty from the TMCMC posterior: the DI field uncertainty is moderate ($\text{DI}_{\text{p95}}/\text{DI}_{\text{p05}} \approx 2$–$3$), translating to ≈ 5–10% stress uncertainty.

4.3 C1. Transverse Isotropy

(All stresses in MPa.)

The dominant *P.g* gradient direction $\mathbf{e}_1$ is approximately $[-0.96, +0.25, -0.14]$ across all conditions (angle ≈ 14–$18°$ from the depth axis x), confirming that *P.g* concentrates near the tooth surface and produces a near-depth anisotropy.

Table 5: C1: S_Mises vs anisotropy ratio β (1 MPa compression)

Condition	$\beta = 1.0$ sub	$\beta = 0.5$ sub	Δ sub	$\beta = 1.0$ surf	$\beta = 0.5$ surf	Δ surf
dh-baseline	0.839	0.817	-2.6%	0.979	0.981	$+0.2\%$
Comm. Static	0.860	0.849	-1.3%	1.020	1.020	0%
Comm. HOBIC	0.854	0.843	-1.3%	1.020	1.020	0%
Dysb. Static	0.856	0.849	-0.8%	1.020	1.020	0%

Reducing β (transverse softer than depth direction) decreases substrate stress by 1–3%. The modest effect is consistent with the small transverse-to-axial modulus contrast at these DI levels.

4.4 Dominant Anisotropy Directions

Table 6: C1: Dominant $\nabla\varphi_{Pg}$ direction per condition

Condition	$\mathbf{e}_1$	Angle from x
dh-baseline	$[-0.972, +0.211, -0.105]$	13.6°
Comm. Static	$[-0.956, +0.258, -0.142]$	17.1°
Comm. HOBIC	$[-0.959, +0.245, -0.145]$	16.5°
Dysb. Static	$[-0.952, +0.262, -0.160]$	17.9°

5 Abaqus CAE Scripting Notes

The Abaqus Python environment (invoked via `abaqus cae noGUI=...`) uses an embedded Python 2-like interpreter with several API quirks. Table ?? lists the issues encountered and their fixes.

Table 7: Abaqus CAE API issues and fixes

Issue	Fix
`math.sqrt(sum(v*v for v in e1))` raises TypeError (generator not accepted)	Replace with explicit: `math.sqrt(e1x*e1x + e1y*e1y + e1z*e1z)`
`mat.Elastic(type="ENGINEERING CONSTANTS")` raises TypeError	Use constant: `mat.Elastic(type=ENGINEERING_CONSTANTS, ...)`
`Region(cells=[cell])` raises TypeError (expects GeomSequence)	Collect element labels per bin; use `part.elements.sequenceFromLabels(labels=...)`
`model.DatumCsysByThreePoints(...)` raises AttributeError	Use `part.DatumCsysByThreePoints(...)` to create datum on the part
`model.fieldOutputRequests["F-Output-1"]` on new model raises KeyError	Remove; default field output is sufficient
Material orientation	`part.MaterialOrientation(region=..., orientationType=SYSTEM, axis=AXIS_1, localCsys=...)`

6 Directory and File Organization

After cleanup (2026-02-21), the FEM root contains:

- **36 Python source files** (no subdirectory nesting needed)
- **Output directories** prefixed with `_` (e.g., `_di_credible`, `_aniso_sweep`)
- `_job_archive/`: 1331 archived Abaqus job files (`.odb`, `.inp`, `.com`, `.dat`, `.msg`, `.prt`, `.sta`, `.log`)
- **2 LaTeX reports**: `fem_report.pdf`, `abaqus_implementation_report.pdf`

7 References

1. P. Wriggers & T. Junker (2024). *A Hamilton principle-based model for diffusion-driven biofilm growth.* Computer Methods in Applied Mechanics and Engineering, CMAME.
2. T. Junker & D. Balzani (2021). *Hamilton principle-based biofilm mechanics model.*
3. Abaqus Documentation (2022). **ELASTIC, TYPE=ENGINEERING CONSTANTS – Transversely isotropic elasticity.*