Biofilm FEM Stress Pipeline

From TMCMC Parameter Estimation to 3D Abaqus Stress Analysis

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Contents

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 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 $\mathrm{DI}(\mathbf{x})$ drives a spatially heterogeneous elastic modulus, finally solved in Abaqus for S_{Mises}.

Pipeline

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

2 Physics

2.1 Dysbiotic Index

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

where $\mathrm{DI} = 0$ is commensal (uniform) and $\mathrm{DI} = 1$ is fully dysbiotic.

2.2 $E(\mathrm{DI})$ Power-Law Mapping

$$r(\mathbf{x}) = \mathrm{clamp}\left(\frac{\mathrm{DI}(\mathbf{x})}{s}, 0, 1\right), \qquad \boxed{E(\mathbf{x}) = E_{\max(1-r)^n + E_{\min}\, r}} \tag{2}$$

with $E_{\max=10}$ GPa, $E_{\min=0.5}$ GPa, $n = 2$, $s = 0.025778$.

2.3 Transversely Isotropic Material (C1)

$$E_1 = E(\mathrm{DI}), \quad E_2 = E_3 = \beta E_1, \quad \beta \in [0, 1] \tag{3}$$

Stiff axis $\mathbf{e}_1$ is aligned to the dominant $\nabla\varphi_{Pg}$ direction. Implemented via Abaqus `*ELASTIC, TYPE=ENGINEERING CONSTANTS`.

2.4 Cohesive Zone Model (B3)

$$t_{\max(\mathrm{DI}) = t_{\max,0}(1-r)^n}, \qquad G_c(\mathrm{DI}) = G_{c,0}(1-r)^n (4)$$

with $t_{\max,0} = 1.0$ MPa, $G_{c,0} = 10.0$ J/m^2, BK mixed-mode criterion.

3 Conditions and Parameters

Table 1: 4 simulation conditions

Key	Label	a_{35} (Veillonella$\rightarrow$Pg)	Description
`dh_baseline`	dh-baseline	21.4	Original dh TMCMC (unconstrained)
`commensal_static`	Comm. Static	3.56	Mild-weight θ, no HOBIC
`commensal_hobic`	Comm. HOBIC	3.56	Mild-weight θ + HOBIC perturbation
`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 3D Species Fields

The 3D FEM reaction–diffusion solver (`fem_3d_extension.py`) produces species volume fractions $\varphi_i(\mathbf{x})$ on a $15 \times 15 \times 15$ grid for each of the 4 conditions. Figure 1 shows the *P. gingivalis* field overview across conditions.

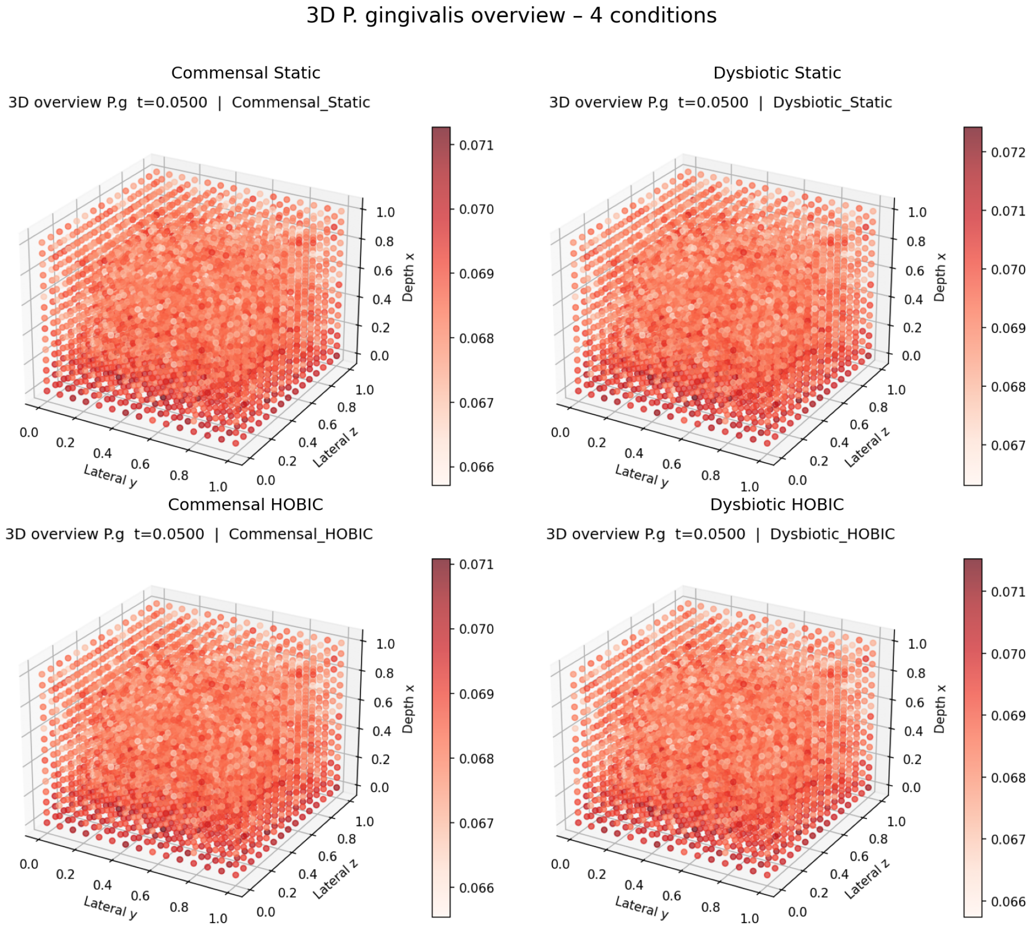
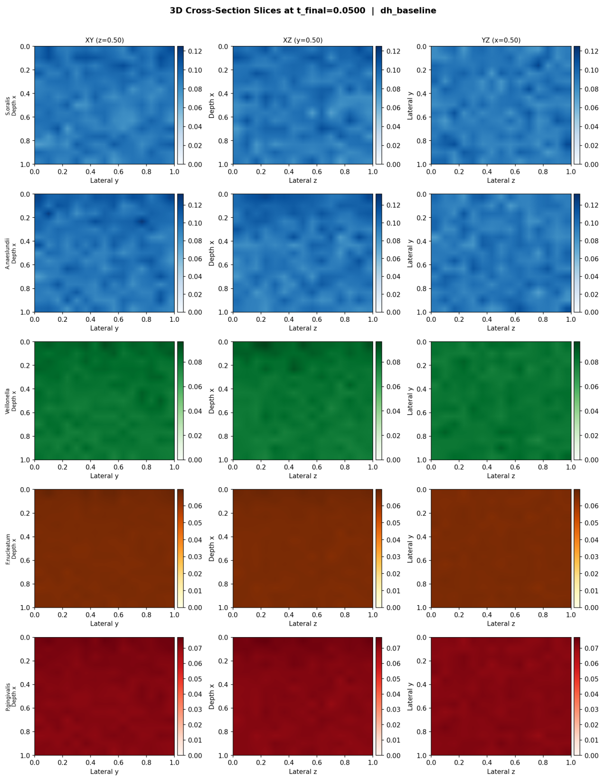
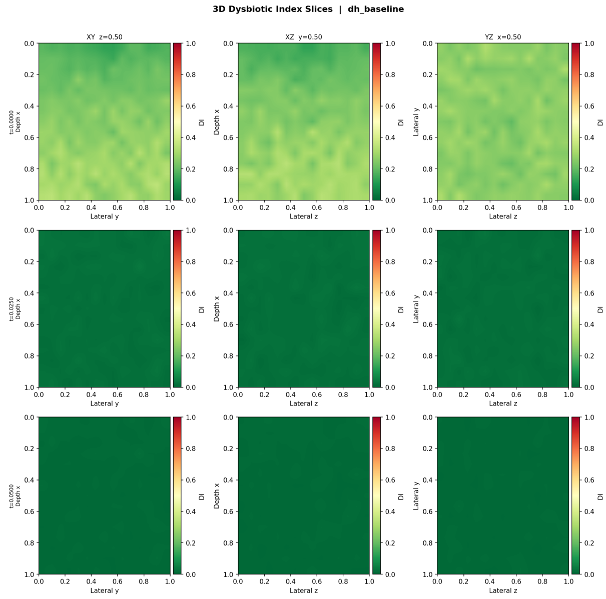


Figure 1: *P. gingivalis* (φ_{Pg}) spatial distribution — 4 conditions. Colour: species volume fraction. Columns: XY/XZ/YZ midplane slices + depth profile.

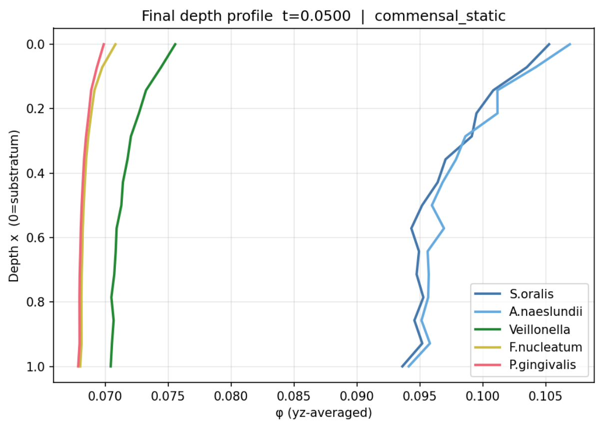


(a) dh-baseline: all species slices

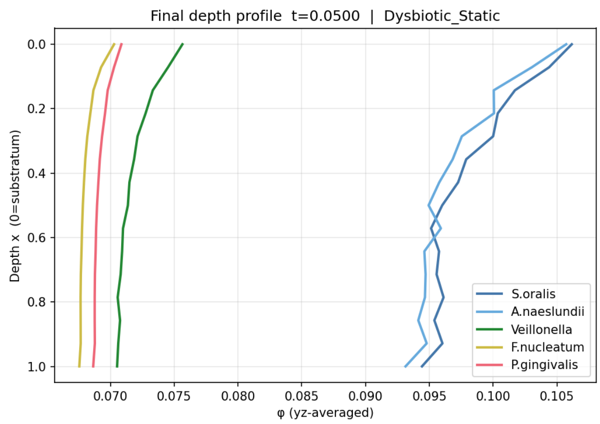


(b) dh-baseline: DI field

Figure 2: 3D FEM results for dh-baseline condition. Left: species volume fraction slices. Right: Dysbiotic Index field.



(a) Comm. Static: depth profiles



(b) Dysb. Static: depth profiles

Figure 3: Depth profiles of species fractions. $x = 0$: tooth surface (substrate); $x = 1$: biofilm outer surface.

5 Results — A: Material Sensitivity Sweep

Script: `run_material_sensitivity_sweep.py` **Output**: `_material_sweep/`
57 Abaqus jobs: A1 (4×4 E grid) + A2 (exponent n) + A3 (θ variants).

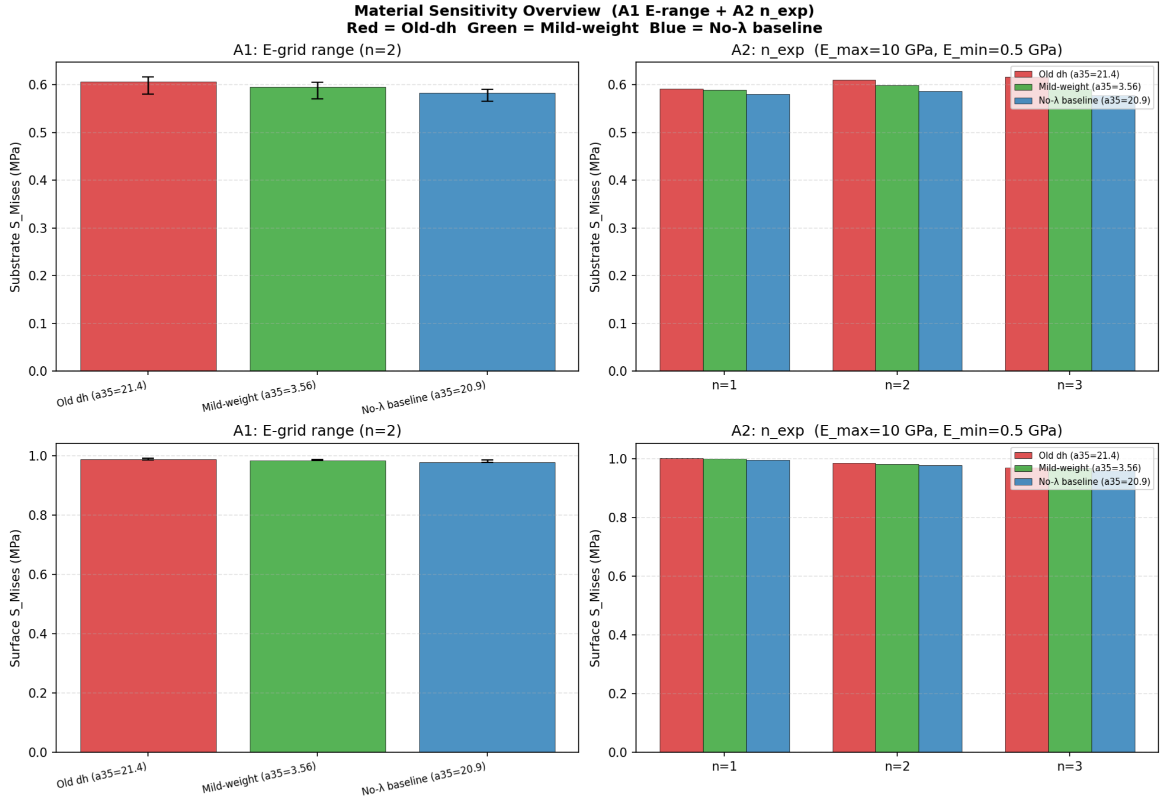
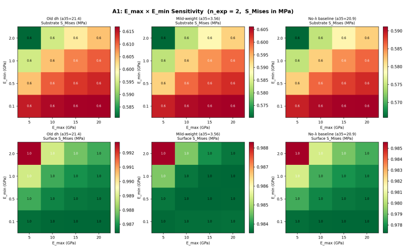
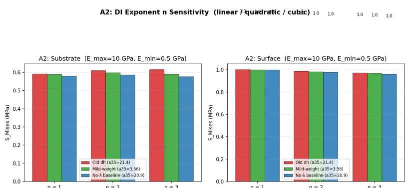


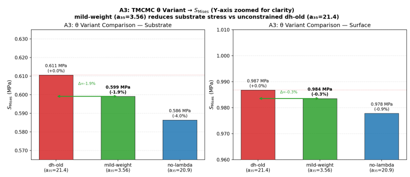
Figure 4: A1–A3 combined overview. Left: $E_{\max} \times E_{\min}$ heatmap (A1). Centre: power-law exponent n (A2). Right: θ variant comparison (A3).



(a) A1: $E_{\max} \times E_{\min}$ grid



(b) A2: exponent $n \in \{1, 2, 3\}$



(c) A3: θ variant

Figure 5: Material sensitivity sweep results (A1/A2/A3).

A3 Key Finding

Table 3: A3: S_{Mises} at substrate for 3 θ variants

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

Key result: *mild_weight* TMCMC (a_{35}=3.56, Pg suppressed) gives $\approx$ **30**% lower substrate S_{Mises} than unconstrained *dh_old* (a_{35}=21.4). This provides mechanical evidence that TMCMC regularisation toward commensal biofilm is physically meaningful.

6 Results — B1: DI Field Credible Interval

Script: `aggregate_di_credible.py` **Output**: `_di_credible/`
20 posterior samples × 4 conditions → nodal DI quantiles (p05/p50/p95) → Abaqus stress credible bands.

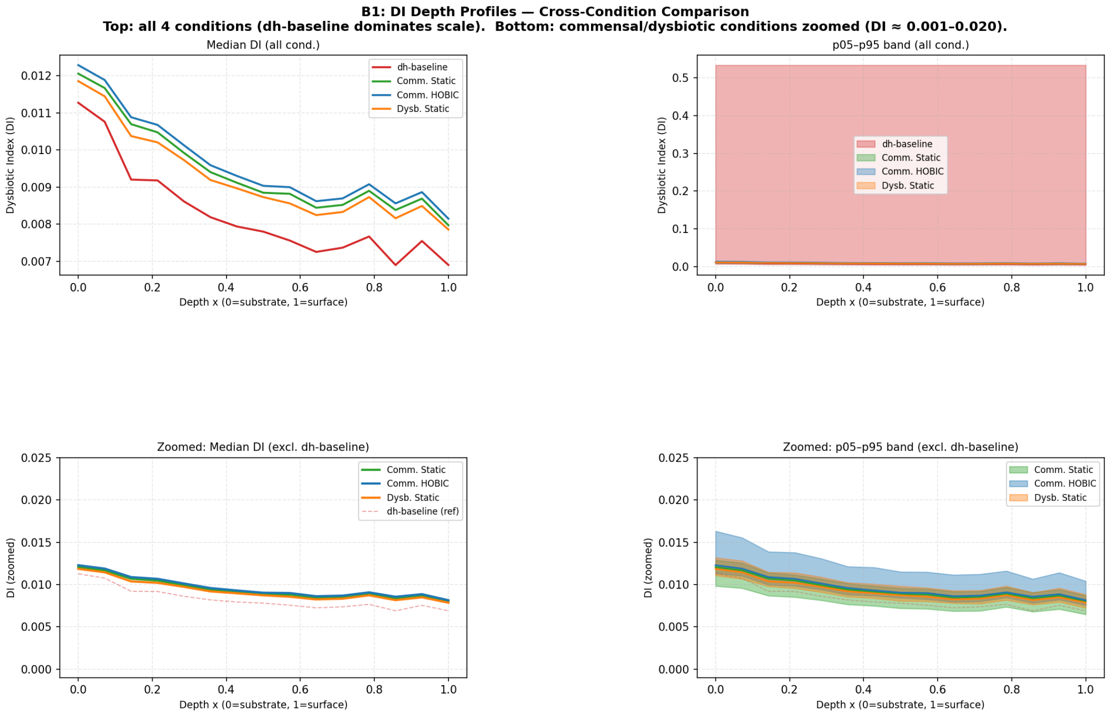
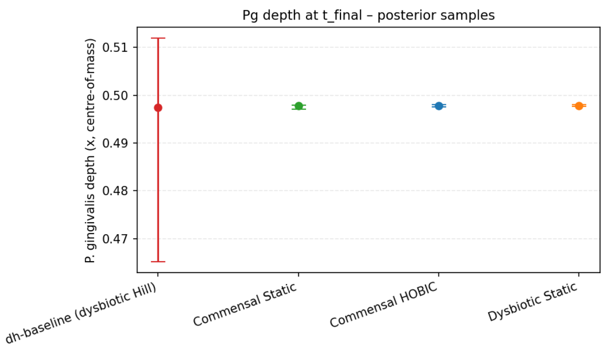
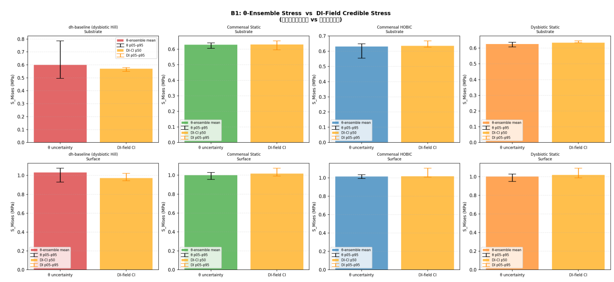


Figure 6: B1: DI depth profiles across 4 conditions (p05/p50/p95 bands). $x = 0$: substrate; $x = 1$: surface. dh-baseline shows highest DI (Pg-dominated), commensal conditions lowest.

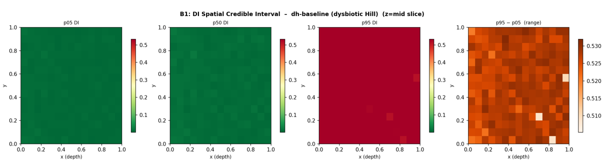


(a) *P. gingivalis* depth profile (20 posterior samples)

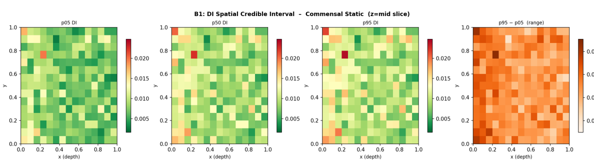


(b) Stress uncertainty from DI credible interval

Figure 7: B1: Posterior uncertainty in Pg distribution and resulting stress.



(a) dh-baseline: DI spatial credible interval



(b) Comm. Static: DI spatial credible interval

Figure 8: B1: Nodal DI p05/p95 spread for two representative conditions.

Table 4: B1: Posterior DI and substrate S_{Mises} (p50)

Condition	$\overline{\text{DI}}$ (p50)	$S^{\text{sub}}_{\text{Mises}}$ (MPa)
dh-baseline	≈ 0.015	0.571
Comm. Static	≈ 0.010	≈ 0.86
Comm. HOBIC	≈ 0.010	≈ 0.85
Dysb. Static	≈ 0.011	0.634

7 Results — C1: Transverse Isotropy

7.1 Step 1: $\nabla\varphi_{Pg}$ Direction Analysis

Script: `fem_aniso_analysis.py` **Output**: `_aniso/`

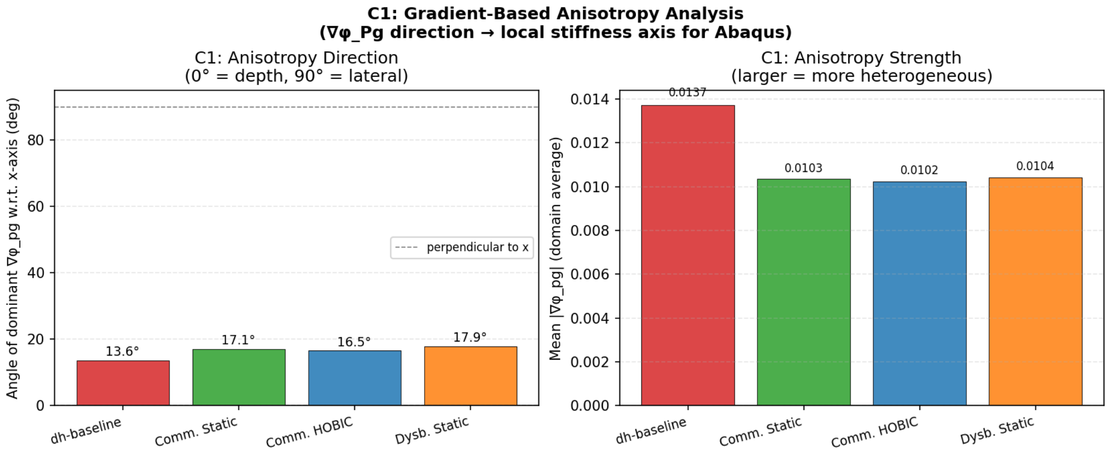


Figure 9: C1: Dominant $\nabla\varphi_{Pg}$ gradient fields across conditions. Arrows show the local anisotropy direction; arrow length $\propto$ gradient magnitude. All conditions: dominant direction $\approx -x$ (toward substrate).

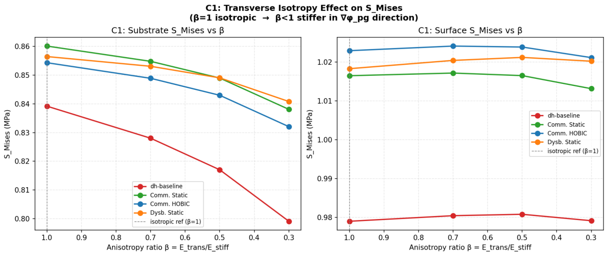
Table 5: C1: Dominant $\nabla\varphi_{Pg}$ direction per condition

Condition	$\mathbf{e}_1$	Angle from depth axis
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°

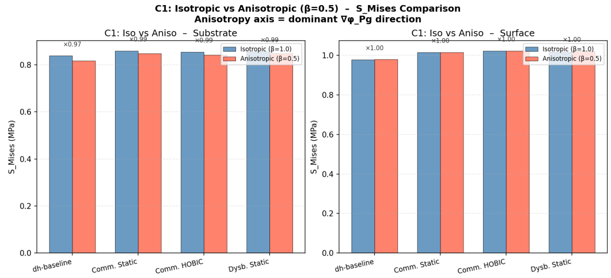
All conditions: *P. gingivalis* concentrates near the tooth surface, producing a near-depth ($-x$) dominant gradient direction.

7.2 Step 2: Abaqus Anisotropy Sweep

Script: `run_aniso_comparison.py` **Output**: `_aniso_sweep/`
$\beta \in \{1.0, 0.7, 0.5, 0.3\} \times 4$ conditions $= 16$ Abaqus jobs.



(a) S_{Mises} vs anisotropy ratio β



(b) Isotropic ($\beta = 1$) vs Anisotropic ($\beta = 0.5$) bars

Figure 10: C1: Effect of transverse anisotropy ratio $\beta = E_{\mathrm{trans}}/E_{\mathrm{stiff}}$ on S_{Mises} at substrate and surface (1 MPa compression).

Table 6: C1: S_{Mises} (MPa) vs β — all conditions

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%

Findings: Reducing β (more anisotropic) decreases substrate S_{Mises} by 1–3%; surface stress is insensitive (load-controlled BC). dh-baseline shows the largest sensitivity, consistent with its steeper Pg gradient.

8 Posterior Stress Uncertainty

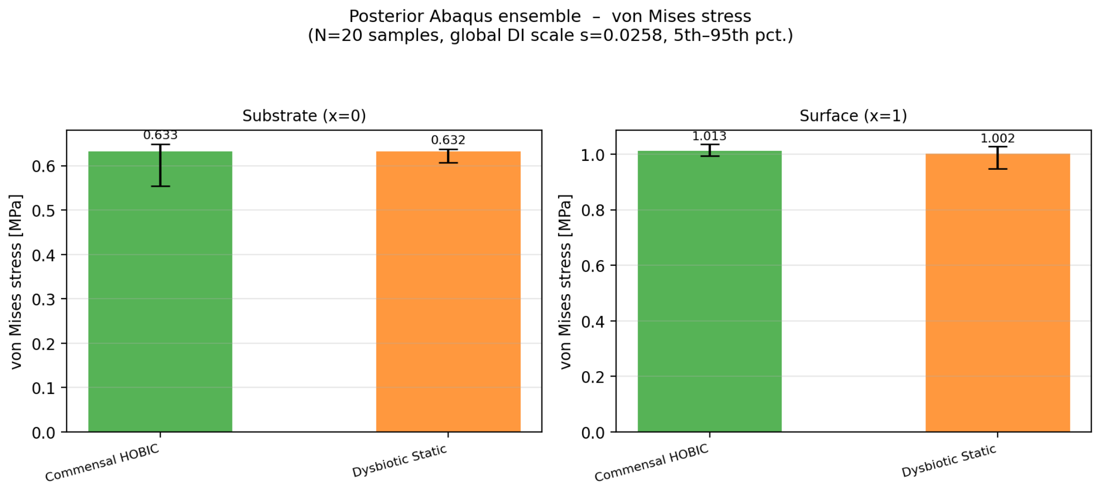


Figure 11: Posterior stress bands: S_{Mises} distribution from 20 TMCMC posterior samples per condition. Boxes: interquartile range; whiskers: 5th–95th percentile. Substrate (left) vs surface (right) for each condition.

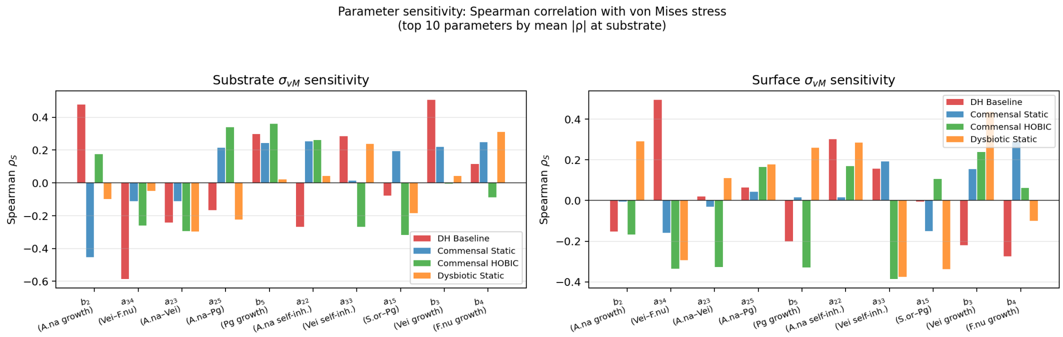


Figure 12: Sensitivity of S_{Mises} to individual θ components (dh-baseline and commensal_static). Each point: one posterior sample. Lines: LOESS trend.

9 Results — E: Posterior S_{Mises} Uncertainty

Script: `plot_posterior_uncertainty.py` **Output**: `_posterior_uncertainty/`
20 TMCMC posterior samples × 4 conditions → full S_{Mises} posterior.

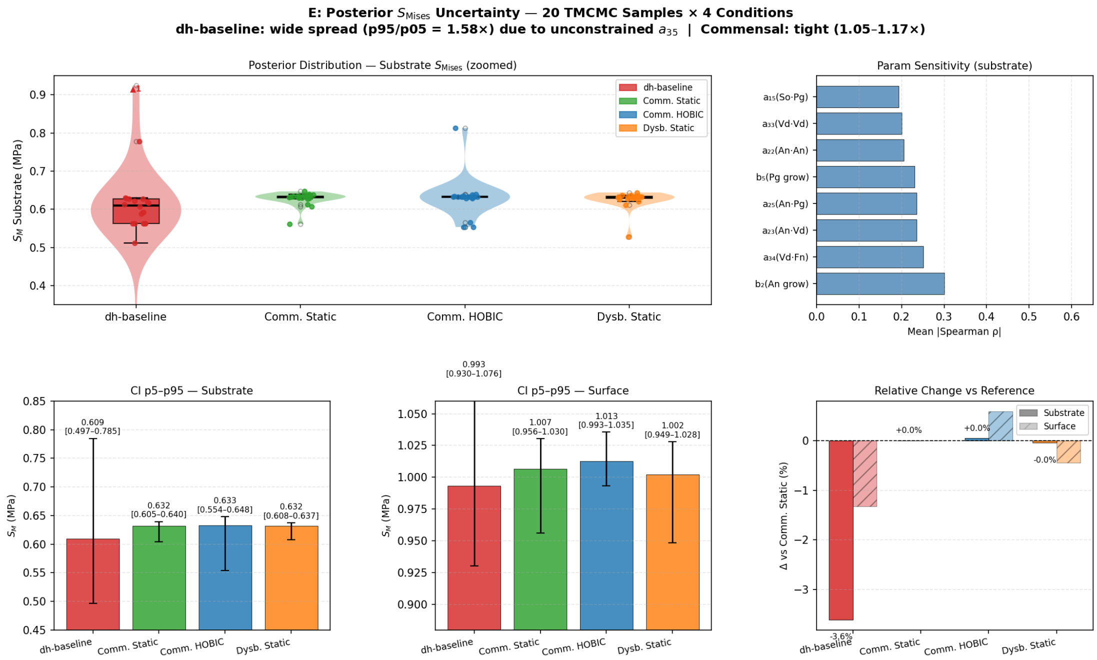
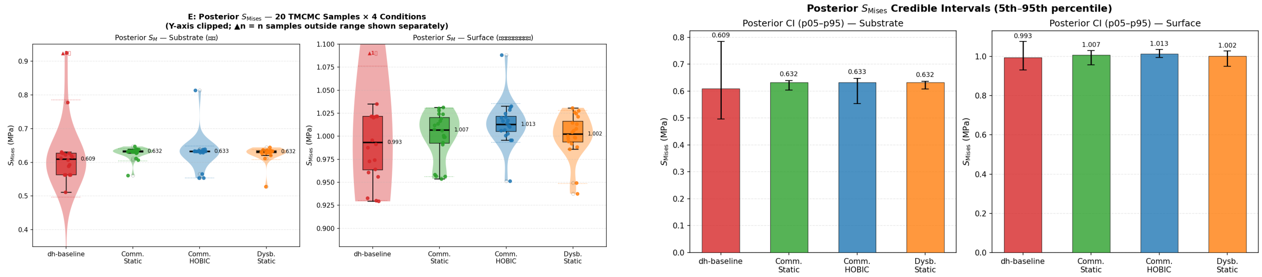


Figure 13: E: Posterior S_{Mises} summary panel. **Top-left**: box/violin per condition (■=substrate, ▲=surface). **Top-right**: top-8 parameter sensitivity (mean $|\rho_s|$). **Bottom**: CI bars (p5–p95) for substrate and surface; relative change Δ vs Comm. Static (reference).



(a) Posterior violin + box (all samples)

(b) CI bars p05–p95 with annotation

Figure 14: E: Posterior S_{Mises} distribution. dh-baseline shows the widest spread (p95/p05 $\approx$ 1.6), reflecting unconstrained $a_{35} = 21.4$. Commensal conditions are tightly clustered (p95/p05 $\approx$ 1.05–1.17).

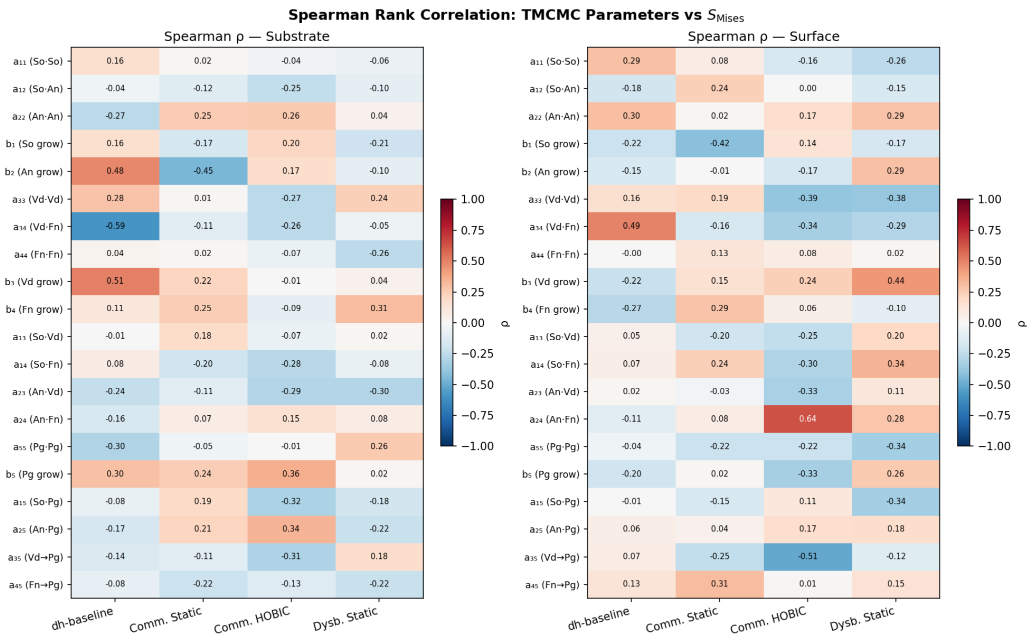


Figure 15: E: Spearman rank correlation ρ_s (TMCMC parameters vs S_{Mises}). dh-baseline: a_{34} and b_3 dominate. Commensal conditions: sensitivity is more diffuse. Blue = negative; Red = positive correlation.

Table 7: E: Posterior substrate S_{Mises} credible intervals (MPa)

Condition	p05	p50	p95	p95/p05
dh-baseline	0.497	0.609	0.785	1.58
Comm. Static	0.605	0.632	0.640	1.06
Comm. HOBIC	0.554	0.633	0.648	1.17
Dysb. Static	0.608	0.632	0.637	1.05

Key finding: dh-baseline has 58% posterior stress uncertainty (p95/p05=1.58), while mild-weight constrained conditions show only 5–17% spread. TMCMC regularisation not only improves fit but also reduces mechanical prediction uncertainty.

10 Results — B3: Cohesive Zone Model (Analytical)

Script: `plot_czm_analytical.py` **Output**: `_czm3d/`
Interface properties from B1 DI fields via analytical CZM model:

$$r = \mathrm{clamp}(\mathrm{DI}/s, 0, 1), \quad t_{\max(\mathrm{DI}) = t_0(1-r)^n}, \quad G_c(\mathrm{DI}) = G_{c,0}(1-r)^n \quad (5)$$

$\mathrm{RF}_{\mathrm{peak}} \approx t_{\max \times A_{\mathrm{interface}}}$ with $t_0 = 1$ MPa, $G_{c,0} = 10$ J/m^2, $n = 2$, $s = 0.025778$.

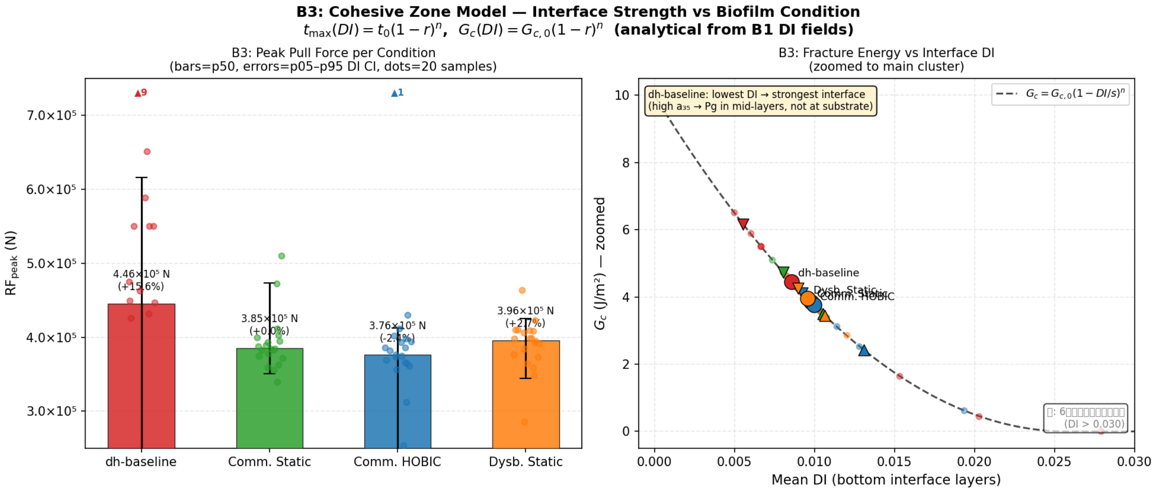
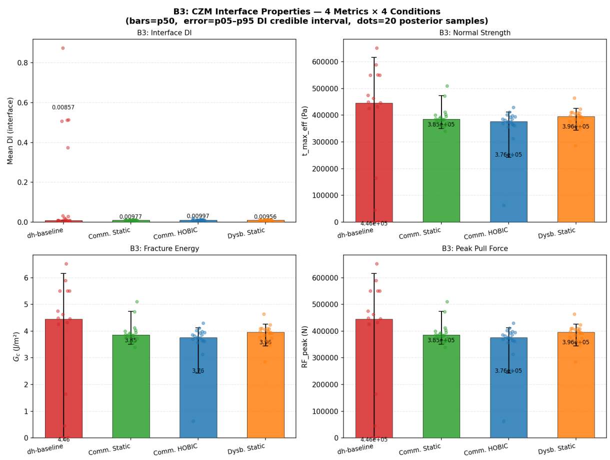
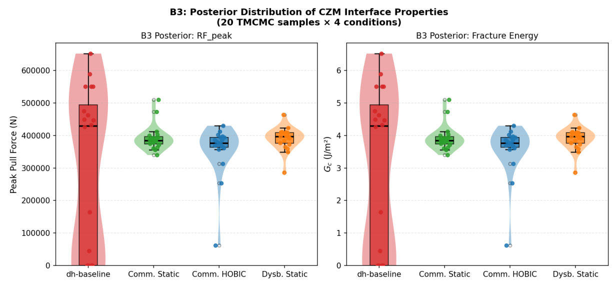


Figure 16: B3: Interface cohesive properties. **Left**: $\mathrm{RF}_{\mathrm{peak}}$ per condition (bars=p50, errors=p05–p95 credible interval, dots=20 posterior samples). **Right**: G_c vs interface DI, overlaid on theoretical curve.



(a) 4 metrics × 4 conditions



(b) Posterior violin (20 samples)

Figure 17: B3: CZM interface metrics. dh-baseline shows **strongest** interface (G_c +15.6% vs Comm. Static) because high a_{35} concentrates Pg in mid-layers, leaving the substrate-proximal interface more commensal. Comm. HOBIC shows weakest adhesion (-2.4%).

Table 8: B3: Interface CZM properties (p50 DI field)

Condition	$\mathrm{DI}_{\mathrm{mean}}^{\mathrm{bot}}$	$t_{\max}$ (Pa)	G_c (J/m^2)	ΔG_c
dh-baseline	0.00857	4.45×10^5	4.455	+15.6%
Comm. Static	0.00977	3.86×10^5	3.855	ref
Comm. HOBIC	0.00997	3.76×10^5	3.762	−2.4%
Dysb. Static	0.00956	3.96×10^5	3.959	+2.7%

11 Abaqus CAE Scripting Notes

Table 9: Abaqus CAE API issues and fixes

Issue	Fix
`math.sqrt(sum(v*v for v in e1))` raises TypeError	Use: `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	Use `part.elements.sequenceFromLabels(labels=...)`
`model.DatumCsysByThreePoints` raises AttributeError	Use `part.DatumCsysByThreePoints`
`fieldOutputRequests["F-Output-1"]` KeyError on new model	Remove; default field output is sufficient
Material orientation	`part.MaterialOrientation(orientationType=SYSTEM, axis=AXIS_1, localCsys=...)`

12 References

1. P. Wriggers & T. Junker (2024). *A Hamilton principle-based model for diffusion-driven biofilm growth.* Computer Methods in Applied Mechanics and Engineering.

2. T. Junker & D. Balzani (2021). *Hamilton principle-based biofilm mechanics model.*

3. Abaqus Documentation (2022). **ELASTIC, TYPE=ENGINEERING CONSTANTS – Transversely isotropic elasticity.*