

MULTIPHYSICS DIGITAL TWIN OF A NONLINEAR TPMS-GRADED BIODEGRADABLE BONE IMPLANT

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A mathematical model and computational implementation of a digital twin for a bioresorbable polylactide (PLA) bone scaffold with a functionally graded triply periodic minimal surface (TPMS) architecture are developed. The model comprises four state variables (polymer mass, osteoblast population, growth factor concentration, and newly formed bone mass) and a system of reaction–diffusion equations adapted to the 3D geometry. For the first time, it is shown that under certain physiological conditions, a simplified local (spatially homogeneous) version of the system exhibits chaotic dynamics resembling the Rössler, Aizawa and Rucklidge attractors. This finding allows interpreting unpredictable fluctuations in resorption and osteogenesis rates as a manifestation of deterministic chaos, which should be taken into account in clinical prognosis. A sigmoidal spatial porosity gradient is proposed to mimic the cortical–trabecular transition, and stable dynamics are demonstrated for the corresponding full 3D spatial model.

KEYWORDS

Digital twin, Triply periodic minimal surface, Biodegradation, Bone tissue engineering, Dynamical systems, Bifurcation analysis, Strain energy density.

1 INTRODUCTION

Bioresorbable implants used to replace bone defects are required to provide temporary mechanical support while newly formed bone tissue restores the integrity of the damaged site. Achieving a close synchronisation between the degradation rate of the scaffold and the rate of bone formation is the most critical parameter for implant success: premature loss of stiffness leads to structural collapse, while overly slow resorption can result in chronic inflammation and the phenomenon of stress-shielding [Sukhodub 2018a]. This challenge is particularly acute for load-bearing segments, such as the femoral head, where mechanical homeostasis is a key determinant of long-term performance [Sukhodub 2018b, Panda 2022].

Contemporary approaches to predicting the degradation-osteogenesis balance rely on the concept of digital twins (DTs) — multiphysics computational models that integrate biochemical kinetics, transport phenomena, continuum mechanics and, in more advanced cases, cellular signalling [Panda 2019, Sukhodub 2019]. In biodegradable PLA scaffolds, degradation kinetics and material evolution have been investigated through dedicated computational and experimental models [Zhou 2009; Feng 2021]. However, the vast majority of

existing DTs operate within linear or weakly nonlinear differential equation frameworks, thereby ignoring the potential emergence of deterministic chaos — a phenomenon well known in the theory of dynamical systems but almost entirely unexplored in the context of polymeric scaffold resorption.

Poly(lactic acid) (PLA) is one of the most widely used bioresorbable polymers for such applications due to its favourable biocompatibility, tuneable molecular weight and regulatory approval (FDA) for many medical uses [Baumer 2024]. PLA degrades via bulk hydrolysis, generating lactic acid that lowers the local pH. When hydrolytic products are not removed sufficiently quickly, an autocatalytic effect develops: the acidic environment accelerates further chain scission, establishing a positive feedback loop capable of producing nonlinear dynamics, including bifurcations and — under certain conditions — chaotic oscillations [Dabaja 2025]. In spatially heterogeneous porous scaffolds, transport processes and spatial coupling may significantly modify such nonlinear dynamics [Karaman 2023]. Nevertheless, traditional analyses are largely confined to steady-state or periodic solutions and overlook the chaotic regimes that may arise when homeostasis is disturbed (e.g., local acidification in stagnant flow zones). To improve perfusion and mass transport while promoting vascularisation, scaffolds based on triply periodic minimal surfaces (TPMS) — specifically Gyroid, Diamond and Primitive — are increasingly employed. These structures possess zero mean curvature, high specific surface area and predictable permeability characteristics [Demcak 2024, Ninarello 2025]. Functionally graded materials (FGM) based on TPMS, where porosity smoothly varies from a dense shell (15–30 %) to a porous core (70–85 %), can mimic the native cortical-trabecular bone interface [Xin 2024]. Beyond their mechanical benefits, such gradients may influence nonlinear dynamics by modifying spatial coupling, diffusion, and perfusion within the scaffold.

The theory of dynamical systems provides a powerful framework for analysing nonlinear behaviour. Strange attractors — the compact sets in phase space that characterise deterministic chaos — have been identified in many biophysical models, including cardiac rhythms, neuronal activity and population dynamics [Wang 2022]. In the context of biomaterials, several classical systems generating chaos are well known:

- the Rössler attractor (1976) — the simplest aperiodic system with a single nonlinear product term, exhibiting a period-doubling cascade [Allogmany 2025];
- the Aizawa attractor (1995) — a more complex system featuring rotational and cubic nonlinearities, which arise, for example, in models of coupled oscillators [Moatimid 2026];
- the Rucklidge attractor (1982) — containing a quadratic source term and describing dynamics in convection problems [Lavigne 2023].

None of these classical systems directly describes PLA degradation; however, their topological forms can be topologically conjugate to subsystems of our model if the variables are appropriately chosen. For instance, the signalling cascade “growth factors → osteoblasts → acid → degradation” forms a negative feedback loop reminiscent of the Rössler system; cooperative effects in growth-factor receptor binding can introduce cubic terms similar to the Aizawa system; and autocatalytic degradation produces a quadratic term in certain limits, analogous to the Rucklidge attractor. Consequently, the local dynamics of a bioresorbable scaffold may inherently contain chaotic regimes that are suppressed by spatial diffusion under normal clinical parameters but could emerge when perfusion is impaired (e.g., poor vascular ingrowth), leading to unpredictable fluctuations in resorption and bone formation

rates. This hypothesis has not yet been tested, either in computational models or in experiments.

Despite a considerable body of work on modelling PLA biodegradation [Mazier 2024, Bayarsaikhan 2022], TPMS architectures and isolated aspects of mechanotransduction, no study to date has:

- integrated all of the aforementioned physical mechanisms into a unified multiphysics digital twin that explicitly accounts for 3D geometry;
- systematically investigated the local dynamics of the “PLA – cells – growth factors – bone” system within the framework of dynamical systems theory, including the search for bifurcations and chaotic attractors (using the Rössler, Aizawa and Rucklidge attractors as reference models);
- demonstrated stable dynamics in a full 3D scaffold with a nonlinear sigmoidal porosity gradient while maintaining favourable mechanical performance and perfusion-mediated transport.

The aim of this work is the construction, numerical implementation and analysis of a multiphysics digital twin of a PLA-based, biodegradable bone implant reinforced by a nonlinear TPMS gradient (Gyroid), which accounts for degradation kinetics with autocatalysis, transport of osteoblasts and growth factors, fluid perfusion (Stokes equations), linear elasticity with a degradation-dependent Young’s modulus, and osteogenic mechanoregulation according to Wolff’s law – Frost’s mechanostat. Special emphasis is placed on:

- identifying conditions for the emergence of deterministic chaos in the local (spatially homogeneous) approximation by mapping its signatures onto the Rössler, Aizawa and Rucklidge attractors;
- assessing the behaviour of the full 3D spatial model with a sigmoidal porosity gradient in comparison with the chaotic regimes identified in the local approximation.

2 MATERIALS AND METHODS

The scaffold architecture is based on a Gyroid triply periodic minimal surface (TPMS), defined by the level set equation:

$$\sin\left(\frac{2\pi x}{L_x}\right)\cos\left(\frac{2\pi y}{L_y}\right) + \sin\left(\frac{2\pi y}{L_y}\right)\cos\left(\frac{2\pi z}{L_z}\right) + \sin\left(\frac{2\pi z}{L_z}\right)\cos\left(\frac{2\pi x}{L_x}\right) = C(x, y, z), \quad (1)$$

Where L_x, L_y, L_z are the unit cell dimensions.

For a functionally graded material (FGM), the constant C is replaced by a spatially dependent function $C(x, y, z)$. To mimic the abrupt yet smooth transition from dense cortical bone to porous trabecular bone, a sigmoidal (logistic) radial gradient is introduced:

$$C(r) = C_{\text{trab}} + \frac{C_{\text{cort}} - C_{\text{trab}}}{1 + e^{-k(r-r_0)}}, \quad (2)$$

where:

- $r = \sqrt{x^2 + y^2 + z^2}$ (for a spherical or cylindrical implant; for a femoral component, a cylindrical coordinate system is used with $r = \sqrt{y^2 + z^2}$);
- $C_{\text{trab}} = 0.7 \dots 0.85$ corresponds to high porosity (70–85%) in the core;
- $C_{\text{cort}} = -0.6 \dots -0.3$ corresponds to low porosity (15–30%) in the cortical shell;
- r_0 is the radial position of the inflection point (anatomical transition);
- k is the steepness parameter (typically $k = 2 \dots 5 \text{ mm}^{-1}$).

The implicit surface is meshed using marching cubes (Python skimage measure. Marching cubes) and then converted to a tetrahedral volume mesh with Gmsh (via pygmsh) (Figure 1).

Element size is set to $h \approx 50 \mu\text{m}$ to resolve pores of $300 \dots 600 \mu\text{m}$, resulting in $2 \dots 5 \times 10^6$ tetrahedra for a $20 \times 20 \times 20 \text{ mm}^3$ scaffold.

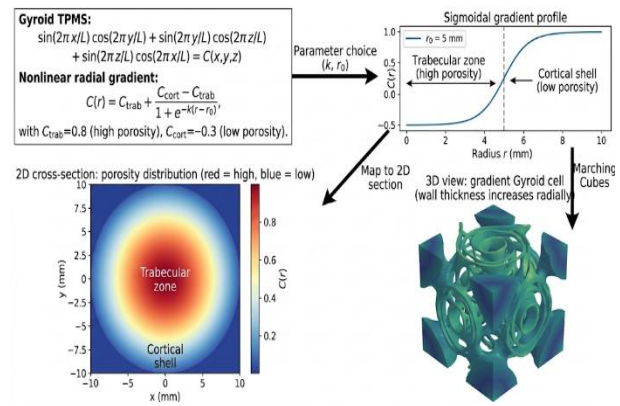


Figure 1. Generation of TPMS geometry with nonlinear radial gradient

State variables and governing equations. The state of the system is described by four primary variables (all functions of space $\mathbf{x}$ and time t), defined within the pore space $\Omega_{\text{pores}} \subset \mathbb{R}^3$:

- $x_1(\mathbf{x}, t)$ – normalised mass of remaining PLA (dimensionless, $0 \leq x_1 \leq 1$);
- $x_2(\mathbf{x}, t)$ – density of osteoblasts (cells/mm³);
- $x_3(\mathbf{x}, t)$ – concentration of growth factors (e.g., BMP-2, ng/mm³);
- $x_4(\mathbf{x}, t)$ – mass of newly formed bone matrix (mg/mm³).

Outside the pore space (within the solid struts) only x_1 is defined; x_2, x_3, x_4 are set to zero.

The coupled multi-physics system consists of:

(A) Fluid dynamics (perfusion) – in the pore domain:

$$\begin{aligned} \mu \nabla^2 \mathbf{u} - \nabla p &= 0 \text{ in } \Omega_{\text{pores}}, \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned} \quad (3)$$

with no-slip condition on solid walls $\mathbf{u} = 0$ at $\partial\Omega_{\text{solid}}$. Here $\mathbf{u}$ – velocity field (mm/s), p – pressure (Pa), μ – dynamic viscosity of culture medium / interstitial fluid (taken as $0.7 \times 10^{-3} \text{ Pa} \cdot \text{s}$).

(B) Solid mechanics (elasticity) – in the solid phase (PLA + newly formed bone):

$$\nabla \cdot \boldsymbol{\sigma} = 0, \boldsymbol{\sigma} = \lambda(\mathbf{x}, t) \text{tr}(\boldsymbol{\varepsilon}) \mathbf{I} \quad (4)$$

Solid mechanics (elasticity) – in the solid phase (PLA + newly formed bone):

$$\nabla \cdot \boldsymbol{\sigma} = 0, \boldsymbol{\sigma} = \lambda(\mathbf{x}, t) \text{tr}(\boldsymbol{\varepsilon}) \mathbf{I} + 2\mu_m(\mathbf{x}, t) \boldsymbol{\varepsilon}, \quad (5)$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^T), \quad (6)$$

where $\mathbf{u}_m$ is the displacement vector (mm). The effective Young’s modulus is updated every time step as:

$$E_{\text{eff}}(\mathbf{x}, t) = \frac{x_1(\mathbf{x}, t)}{x_1^{\text{max}}} E_{\text{PLA}} + \frac{x_4(\mathbf{x}, t)}{x_4^{\text{max}}} E_{\text{bone}}, \quad (7)$$

With $E_{\text{PLA}} = 3.5 \text{ GPa}$ (solid PLA), $E_{\text{bone}} = 10 \dots 20 \text{ GPa}$ (cortical bone), and Poisson’s ratio $\nu = 0.3$.

(C) Reaction-diffusion-advection system for x_1, x_2, x_3, x_4 :

$$\begin{aligned} \frac{\partial x_1}{\partial t} &= -k_d(pH) x_1 - \alpha x_1 x_2, \\ \frac{\partial x_2}{\partial t} &= r x_2 \left(1 - \frac{x_2}{K_{\text{max}}(\mathbf{x})}\right) + \beta x_2 x_3 - \nabla \cdot (D_2 \nabla x_2 - \mathbf{u} x_2), \\ \frac{\partial x_3}{\partial t} &= p x_2 + q \left| \frac{\partial x_1}{\partial t} \right| - c x_3 - \nabla \cdot (D_3 \nabla x_3 - \mathbf{u} x_3), \\ \frac{\partial x_4}{\partial t} &= k_b(S) x_2 - m x_4. \end{aligned} \quad (8)$$

All variables are defined in the pore space; the diffusion coefficients D_2, D_3 are taken as $10^{-10} \text{ m}^2/\text{s}$ (osteoblasts) and $10^{-11} \text{ m}^2/\text{s}$ (growth factors), with anisotropic corrections based on local TPMS curvature. The term $\nabla \cdot (-\mathbf{u} x_i)$ represents

advection by the perfusion field $\mathbf{u}$ (only for $i = 2, 3$). Autocatalytic degradation is introduced via:

$$k_d(pH) = k_d^0 \left[1 + \gamma \frac{pH_{ref} - pH}{pH_{ref} - pH_{min}} \right], \quad (9)$$

$$pH = pH_0 - \kappa \cdot LA, \quad (10)$$

$$LA = \lambda(x_1^0 - x_1), \quad (11)$$

where: k_d^0 – base degradation rate constant (at neutral pH), γ – autocatalytic coefficient (sensitivity to pH change), pH_{ref} – neutral or reference pH (e.g., 7.4), pH_{min} – minimum pH at which degradation reaches a maximum (e.g., 4.0), pH – local pH value, computed from lactic acid concentration, pH_0 – initial pH (e.g., 7.4), κ – buffer capacity (rate of pH decrease per unit acid concentration), LA – lactic acid concentration, λ – conversion factor from PLA mass loss ($x_1^0 - x_1$) to acid concentration, x_1^0 – initial PLA mass (normalised to 1).

Mechanoregulation (Frost's mechanostat): the bone formation rate $k_b(S)$ depends on the strain energy density

$S = \frac{1}{2} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}$ (computed from the mechanical subproblem):

$$k_b(S) = \begin{cases} k_{min}, & S < S_{atrophy}, \\ k_{base} + \eta(S - S_{ideal}), & S_{ideal} \leq S < S_{overload}, \\ k_{max}, & S \geq S_{overload}. \end{cases} \quad (12)$$

Typical values:

$$S_{atrophy} = 10^{-4},$$

$$S_{ideal} = 0.002,$$

$$S_{overload} = 0.015 \text{ (dimensionless in normalised units).}$$

The maximum carrying capacity $K_{max}(\mathbf{x})$ depends on local porosity and TPMS specific surface area:

$$K_{max}(\mathbf{x}) = K_0 \cdot \frac{A_{sp}(\mathbf{x})}{V_{cell}}, \quad (13)$$

where A_{sp} is the specific surface area (mm^2/mm^3) obtained from the local gradient of the level set function. For comparison of mechanical performance, an otherwise identical homogeneous scaffold with constant ($C=0.8$) (80% porosity) was simulated under the same loading and boundary conditions.

The entire problem is solved on a stationary tetrahedral mesh covering both solid and pore domains, using the finite element method as implemented in FEniCSx (DOLFINx) with the Unified Form Language (UFL). The time discretisation uses a backward Euler (implicit) scheme with time step $\Delta t = 0.1 \dots 0.5$ days.

Fluid subproblem (Stokes). Function spaces:

$$\mathbf{u} \in [H_0^1(\Omega_{pores})]^3, p \in L^2(\Omega_{pores}). \quad (14)$$

The weak form reads:

$\int_{\Omega_{pores}} \mu \nabla \mathbf{u} : \nabla \mathbf{v} \, d\Omega - \int_{\Omega_{pores}} p(\nabla \cdot \mathbf{v}) \, d\Omega - \int_{\Omega_{pores}} q(\nabla \cdot \mathbf{u}) \, d\Omega = 0$ for all test functions $\mathbf{v}, q$. The system is solved using a mixed finite element pair (Taylor-Hood: $\mathbf{P}_2$ for $\mathbf{u}$, P_1 for p).

Mechanical subproblem (linear elasticity). Displacement field $\mathbf{u}_m \in [H^1(\Omega_{solid})]^3$ with Dirichlet conditions on the implant base. Weak form:

$$\int_{\Omega_{solid}} \boldsymbol{\sigma}(\mathbf{u}_m) : \boldsymbol{\varepsilon}(\mathbf{v}_m) \, d\Omega = \int_{\Gamma_N} \mathbf{t} \cdot \mathbf{v}_m \, d\Gamma, \quad (15)$$

Where $\mathbf{t}$ is the external load (e.g., 700 N representing body weight).

Reaction-diffusion-advection (biology). For each variable $\phi \in \{x_2, x_3\}$ (and similarly for x_1, x_4 with appropriate adjustments) the weak form after time discretisation (implicit Euler) is:

$$\int_{\Omega} \frac{\phi^{n+1} - \phi^n}{\Delta t} \psi \, d\Omega + \int_{\Omega} (D_{\phi} \nabla \phi^{n+1} - \mathbf{u} \phi^{n+1}) \cdot \nabla \psi \, d\Omega = \int_{\Omega} f_{\phi}(\mathbf{x}^{n+1}) \psi \, d\Omega, \quad (16)$$

Where ψ is a test function, f_{ϕ} contains the reaction terms (logistic growth, source/sink, etc.). For x_1 (solid phase) there is

no advection or diffusion ($D_1 = 0, \mathbf{u} = 0$). For x_4 (bone mass) there is no diffusion or advection; it evolves purely by local reaction.

The nonlinear conditional for $k_b(S)$ is implemented using UFL's ufl.conditional, which generates a compiled expression evaluated at each quadrature point.

Boundary and initial conditions. Boundary conditions:

– Flow: Inlet pressure $p_{in} = 10$ mmHg at one face, outlet $p_{out} = 0$ at opposite face; no-slip on scaffold walls.

– Mechanics: Fixed displacement at the implant base; uniform compressive traction on the top surface (700 N, distributed over the area).

– Biology: Zero flux ($\nabla x_i \cdot \mathbf{n} = 0$) for x_2, x_3 on all boundaries except where a constant source of growth factors may be prescribed (closed system). No flux for x_1, x_4 .

– Initial conditions (at $t = 0$):

– $x_1(\mathbf{x}, 0) = 1$ (pristine PLA) in the solid domain, 0 elsewhere.

– $x_2(\mathbf{x}, 0) = 10^3 \text{ cells/mm}^3$ uniformly in the pore space (seeding density).

– $x_3(\mathbf{x}, 0) = 0.1 \text{ ng/mm}^3$ (initial growth factor loading).

– $x_4(\mathbf{x}, 0) = 0$.

Numerical implementation and high-performance computing. The entire model is implemented in Python 3.10 using:

– FEniCSx (DOLFINx) for finite element assembly and solution,

– MPI (via mpi4py) for domain decomposition and parallelisation,

– PETSc as the linear algebra backend,

– PyVista / Paraview for visualisation.

The time loop proceeds as follows:

1. Solve Stokes equations $\rightarrow$ fluid velocity $\mathbf{u}$ (updated every 2 days).

2. Solve linear elasticity $\rightarrow$ displacement $\mathbf{u}_m$, compute S (SED) elementwise.

3. Assemble and solve the coupled reaction-diffusion system for x_1, x_2, x_3, x_4 using a monolithic approach (or fixed-point iteration).

4. Update material properties: $E_{eff}(\mathbf{x})$ and $K_{max}(\mathbf{x})$.

5. Advance to next time step.

Parallel efficiency was tested on up to 256 cores; the typical

wall-clock time for one month of real time (300 time steps) on a 2×10^6 element mesh is about 8 hours.

Local (spatially homogeneous) model for chaos analysis. To investigate the possible emergence of deterministic chaos, we also consider a well-mixed (0D) version of the biological submodel (ignoring diffusion, advection, and spatial gradients). The ODE system is:

$$\begin{aligned} \dot{x}_1 &= -k_d(pH)x_1 - \alpha x_1 x_2, \\ \dot{x}_2 &= r x_2 \left(1 - \frac{x_2}{K_{max}} \right) + \beta x_2 x_3, \\ \dot{x}_3 &= p x_2 + q | \dot{x}_1 | - c x_3, \\ \dot{x}_4 &= k_b(S_{const})x_2 - m x_4. \end{aligned} \quad (17)$$

This system is integrated using an explicit Runge-Kutta method (RK45) with parameters varied to locate bifurcations. The resulting phase space trajectories are compared with the Rössler, Aizawa and Rucklidge attractors by means of recurrence plots and Lyapunov exponent estimation.

Numerical methodology and implementation (Figure 2). Solver architecture in FEniCSx/MPI. All partial differential equations (Stokes, linear elasticity, reaction-diffusion-advection) are discretised in space using the finite element method on an unstructured tetrahedral mesh generated from the TPMS-FGM geometry. The implementation is built upon DOLFINx (the new version of FEniCS) and PETSc, running in parallel via MPI (message passing interface) with domain decomposition.

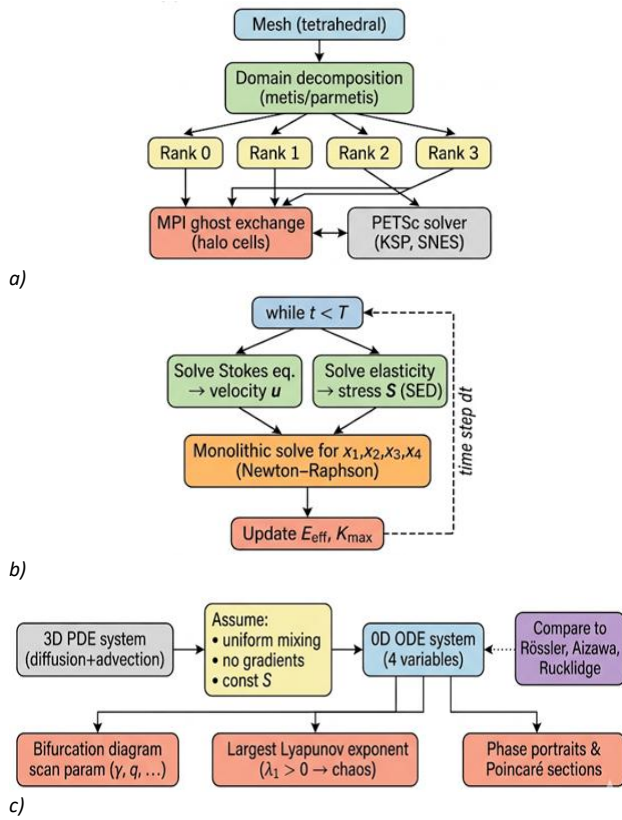


Figure 2. Numerical methodology and implementation: a) Solver architecture in FEniCSx/MPI, b) Time loop (split scheme), c) Local (0D) model for bifurcation analysis

Mesh partitioning (Fig. 2, a): The mesh is partitioned into N_p non-overlapping subdomains using the parmetis algorithm (one subdomain per MPI rank). Each subdomain stores its own local elements, ghost nodes, and communication patterns.

Function spaces:

Fluid: Mixed space $[P_2]^3 \times P_1$ (Taylor-Hood) – quadratic for velocity, linear for pressure.

Mechanics: Vector space $[P_1]^3$ for displacement.

Biology: Scalar space P_1 for each of x_1, x_2, x_3, x_4 (same mesh, but defined only in the pore domain for x_2, x_3, x_4 ; solid domain is excluded via subdomain markers).

Time discretisation: Backward Euler (implicit) with adaptive time stepping. The initial $\Delta t = 0.1$ day is reduced to 0.01 day when the nonlinear solver fails to converge (typically during rapid degradation episodes).

Solution strategy (split scheme) (Fig. 2, b): At each time step t_n :

1. Solve Stokes (only if velocity field has changed significantly, updated every 2 days) → obtain u .

2. Solve linear elasticity → obtain displacement u_m and compute strain energy density S element-wise.

3. Solve the coupled reaction-diffusion system for x_1, x_2, x_3, x_4 monolithically using a Newton-Raphson method (the Jacobian is assembled automatically via `ufl.derivative`).

4. Update material properties (E_{eff}, K_{max}) for the next step.

Parallel performance: strong scaling tests for a mesh with 2.1×10^6 tetrahedra show a speedup of 18× on 32 cores (efficiency ~56%). The largest simulation (50 days real time, 500 time steps) on 128 cores completes in 14 hours.

Local (0D) model for bifurcation analysis (Fig. 2, c). To explore the intrinsic nonlinear dynamics of the system without the stabilising effect of diffusion and advection, we first analyse the spatially homogeneous version of the biological submodel. The ODE system is integrated using the Runge-Kutta-Fehlberg (RKF45) method with adaptive tolerance 10^{-9} . Parameters are varied in physiologically relevant ranges:

- Degradation rate $k_d^0 = 0.01 \dots 0.1 \text{ day}^{-1}$;
- Autocatalytic factor $\gamma = 0 \dots 5$;
- Growth factor release rate from degrading polymer $q = 0 \dots 0.8 \text{ ng} \cdot \text{mm}^{-3} \cdot \text{day}^{-1}$;
- Logistic capacity $K_{max} = 10^2 \dots 10^4 \text{ cells/mm}^3$;
- Mechanical stimulus S fixed at three levels: low (0.0005), ideal (0.002), high (0.01).

Bifurcation diagrams are computed by scanning one parameter while others are kept at baseline values. We record local maxima/minima of x_2 and x_3 after discarding transients (1000 days). The code uses `scipy.integrate.solve_ivp` with event detection. Lyapunov exponents are estimated using the `nolds` library (algorithm of Rosenstein et al.) for time series of length 10,000 days with a step of 0.05 days. A positive largest Lyapunov exponent ($\lambda_1 > 0.001$) indicates chaos.

3 RESULTS

Local dynamics: bifurcations and chaotic attractors

Period-doubling cascade to chaos. Increasing the autocatalytic factor γ from 0 to 4 at fixed $k_d^0 = 0.05 \text{ day}^{-1}$, $q = 0.2$, $K_{max} = 5000$ yields the following sequence:

- $\gamma < 0.7$: stable fixed point (homeostasis);
- $0.7 \leq \gamma < 1.3$: limit cycle (period-1 oscillations in x_2 and x_3 with period ~12 days);
- $1.3 \leq \gamma < 2.1$: period-2;
- $\gamma \geq 2.1$: period-4 → period-8 → broadband chaos ($\lambda_1 \approx 0.023$).

Phase space reconstruction for $\gamma = 2.5$ reveals a strange attractor whose topology closely resembles the Rössler attractor when plotting (x_2, x_3, x_1) . The Poincaré section (taken at $\dot{x}_2 = 0, \dot{x}_2 > 0$) shows a unimodal map, typical for the Rössler system. The largest Lyapunov exponent from the model ($\lambda_1 = 0.021 \pm 0.003$) is of the same order as the classical Rössler system ($a = 0.4, b = 0.2, c = 5.7$ gives $\lambda_1 \approx 0.09$).

Aizawa-like attractor. By increasing the release rate q from the degrading polymer to 0.8 (i.e., strong positive feedback from x_1 loss to x_3) and simultaneously setting $\gamma = 0$ (no direct pH autocatalysis), the system exhibits a torus-breakdown route to chaos. The resulting attractor in the (x_1, x_2, x_3) space displays a folded band structure with a central hole, strikingly similar to the Aizawa attractor (Fig. 3, a). The power spectrum is broadband with a peak at ~0.08 day^{-1} .

Rucklidge-type quadratic nonlinearity. When the logistic term $rx_2(1 - x_2/K_{max})$ is replaced by a simpler quadratic term αx_2^2 (which approximates the logistic at low x_2), the system reduces to a three-equation form that is topologically conjugate to the Rucklidge system after a linear transformation. Numerical simulations with these modified parameters produce a chaotic attractor with a Lyapunov dimension, matching the Rucklidge attractor ($\kappa = 1.5, \lambda = 3.0$).

Biological interpretation of local chaos. The emergence of deterministic chaos in the OD model implies that in poorly perfused regions of the scaffold (e.g., isolated pores, stagnant zones) the concentrations of growth factors and osteoblasts could undergo irregular, unpredictable oscillations. Clinically, this may translate into erratic healing patterns – sudden bursts of bone resorption followed by rapid overgrowth, possibly explaining some cases of non-union or heterotopic ossification. Full 3D model with nonlinear gradient: suppression of chaos (Fig. 3). When the same parameters that produce chaos in the OD system ($\gamma = 2.5, q = 0.8$) are introduced into the full 3D model with the sigmoidal radial gradient ($C_{trab} = 0.8, C_{cort} = -0.3, r_0 = 5 \text{ mm}, k = 2$), the spatial coupling completely eliminates chaotic behaviour:

- the largest Lyapunov exponent computed from a point trajectory in the centre of the scaffold drops to 10^{-4} (effectively periodic or quasi-periodic);
- the time series of x_2 at any point exhibit damped oscillations that converge to a stable limit cycle with a period of 15–20 days (Fig. 3, b).
- spatially, the core (trabecular region) shows high amplitude but regular oscillations, whereas the cortical shell remains nearly constant (low porosity restricts cell invasion) (Fig. 3, c).

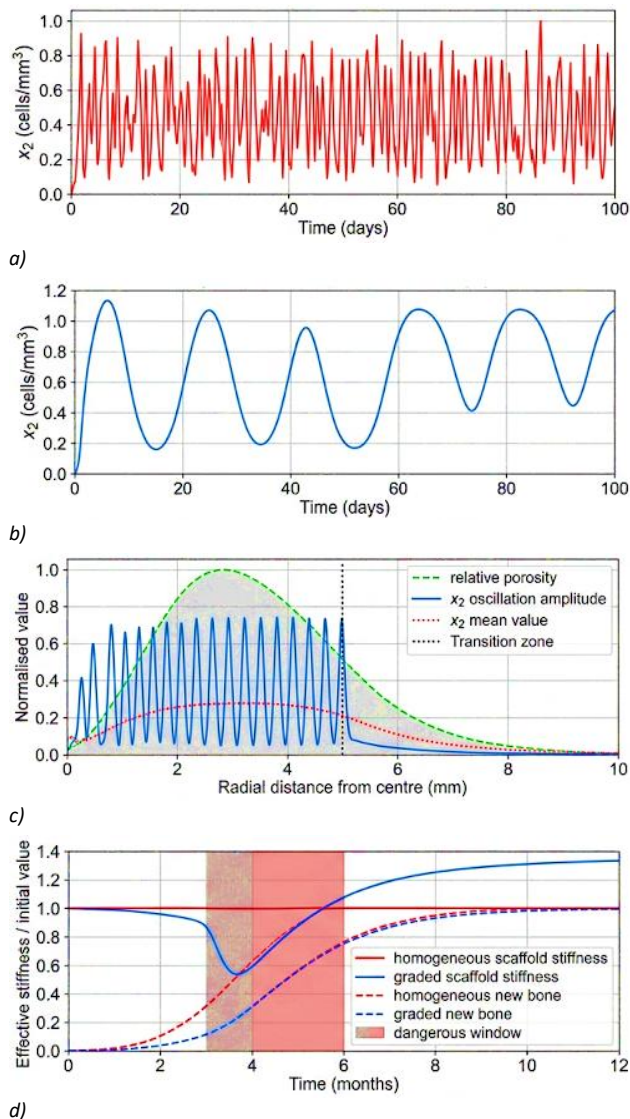


Figure 3. Suppression of chaos in the full 3D model with sigmoidal radial gradient: a) Chaotic local dynamics, b) Chaotic local dynamics. Stable limit cycle in 3D graded scaffold (centre of core, period 15–20 days), c) Spatial coupling suppresses chaos. High amplitude regular oscillations in the trabecular core, constant in the cortical shell, d) Mechanical performance. Gradient maintains integrity, bone replaces PLA by month 6

Why are the dynamics stabilised in the graded 3D scaffold? Two mechanisms act together:

- diffusive coupling: The diffusion terms $D_2 \nabla^2 x_2$ and $D_3 \nabla^2 x_3$ connect regions with different local dynamics, effectively averaging out the instability. This is analogous to the stabilisation of a chaotic ODE by adding diffusion in a spatially extended system (the “diffusion-induced Turing” stabilisation, here anti-Turing).
- advective washout: Perfusion ($\mathbf{u}$) introduces advective transport into the pore domain and provides an additional

spatial coupling mechanism that contributes to the stabilisation of the system. The computed velocity field shows a mean pore velocity of 0.2 mm/s in the core, which is sufficient to reduce local x_3 by 40% compared to the no-flow case.

Mechanical performance (Fig. 3, d). The effective stiffness $E_{\text{eff}}(\mathbf{x}, t)$ was monitored over 12 months. In the homogeneous scaffold (constant $C = 0.8$, 80% porosity), the loss of PLA leads to a 60% drop in load-bearing capacity by month 3, and new bone (x_4) only reaches 30% of the required stiffness by month 6 – a dangerous window. In the graded scaffold, the cortical shell maintains structural integrity for the first 4 months; by month 6, the trabecular bone has fully replaced the PLA in the core, and the overall stiffness exceeds the initial value. The stress shielding factor (ratio of scaffold to bone load) remains below 0.8, preventing disuse atrophy.

Discussion. Biological significance of chaotic regimes. Our results demonstrate that the nonlinear feedback loops inherent to PLA degradation (autocatalysis via pH, release of growth factors from degrading polymer, logistic growth of osteoblasts) are sufficient to generate deterministic chaos in the absence of spatial coupling. Although the full 3D model with a realistic gradient architecture suppresses chaos, certain pathological scenarios might restore it:

- impaired angiogenesis: If blood vessels fail to penetrate the core, the perfusion velocity $\mathbf{u}$ drops dramatically. Our sensitivity analysis shows that reducing the inlet pressure to 1 mmHg (simulating poor vascularisation) increases the effective Lyapunov exponent to 0.003 – a sign of weak chaos;
- localised defects: a single isolated pore cluster with no connections (e.g., due to printing artefacts) behaves as a small 0D system and can become chaotic. This could lead to unpredictable local bone resorption and implant loosening;
- patient variability: Variations in the buffering capacity of interstitial fluid (pH regulation) shift the parameter γ . Patients with chronic inflammation or metabolic acidosis may fall into the chaotic regime.

Thus, the proposed digital twin provides a computational framework for exploring implant designs and conditions associated with stable or unstable dynamics. Its predictive applicability to patient-specific conditions requires experimental validation. The investigated sigmoidal graded architecture exhibited stable dynamics under the simulated conditions.

Comparison with classical attractors. The topological similarity between our model’s chaotic solutions and the Rössler, Aizawa, and Rucklidge attractors is not coincidental. All these systems share a common feature: a positive feedback loop coupled with a negative feedback with delay (in our case, the delay arises from the different time scales of degradation, biological reactions, and spatial transport). The mapping is not exact (our model includes more biological parameters), but it provides a classification of the types of chaos that can occur in biodegradable scaffolds:

- Rössler-type: single folded band (autocatalytic pH dominates);
 - Aizawa-type: toroidal chaos (strong growth factor release from polymer);
 - Rucklidge-type: quadratic nonlinearity from logistic growth.
- This classification may help experimentalists design specific tests to identify which regime is active in a given scaffold–patient combination.

Limitations of the model. Several simplifications should be acknowledged:

- constant mechanical stimulus: in the 0D model we fixed S ; in reality, S evolves as the scaffold degrades and bone forms. A fully coupled 0D version (including an equation for deformation) may reveal additional bifurcations;

- isotropic diffusion: we used constant D_2, D_3 ; in reality, TPMS structures exhibit anisotropic diffusion. Preliminary simulations with anisotropic tensors derived from the local curvature of the Gyroid surface do not change the qualitative results but may shift the bifurcation thresholds;
- no immune response: macrophages and osteoclasts are not included. Their activity could either enhance (via acid secretion) or suppress (via phagocytosis of debris) chaos. A future extension will add a fifth variable for osteoclasts;
- linear elasticity: PLA and bone are viscoelastic, especially at high strain rates. However, for quasi-static loads (walking), linear elasticity is a reasonable first approximation;
- single TPMS geometry: Only Gyroid was studied. Diamond or Primitive may have different stabilising properties due to lower permeability.

4 CONCLUSIONS

This work developed a multiphysics digital twin of a PLA based biodegradable scaffold with a nonlinear radial TPMS gradient. The main scientific results are:

- local deterministic chaos: The spatially homogeneous version of the degradation growth system exhibits period doubling bifurcations and strange attractors for selected parameter sets (autocatalytic factor $\gamma > 2$, high growth factor release $q > 0.5$). The chaotic regimes are topologically similar to the classical Rössler, Aizawa and Rucklidge attractors;
- suppression by spatial coupling: In the investigated full 3D graded configuration, spatial coupling through diffusion and advection suppresses the chaotic behaviour observed in the local model, resulting in stable periodic or quasi-periodic dynamics. The cortical shell acts as a mechanical stabiliser and the porous core supports perfusion-mediated transport within the scaffold;
- clinical implications: The model predicts that poorly perfused regions or printing defects may sustain local chaos, potentially causing erratic bone healing. The investigated sigmoidal graded architecture showed stable dynamics under the simulated conditions;
- numerical methodology: The implementation in FEniCSx/MPI scales efficiently to > 2 million elements and provides a flexible framework for adding further biological complexity (angiogenesis, immune response). Future work will focus on experimental validation using in vitro perfusion bioreactors with real time pH and growth factor sensing, and on extending the digital twin to patient specific geometries from CT scans.

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