Numerical simulation of biodegradation and corrosion of magnesium-based orthopedic implants

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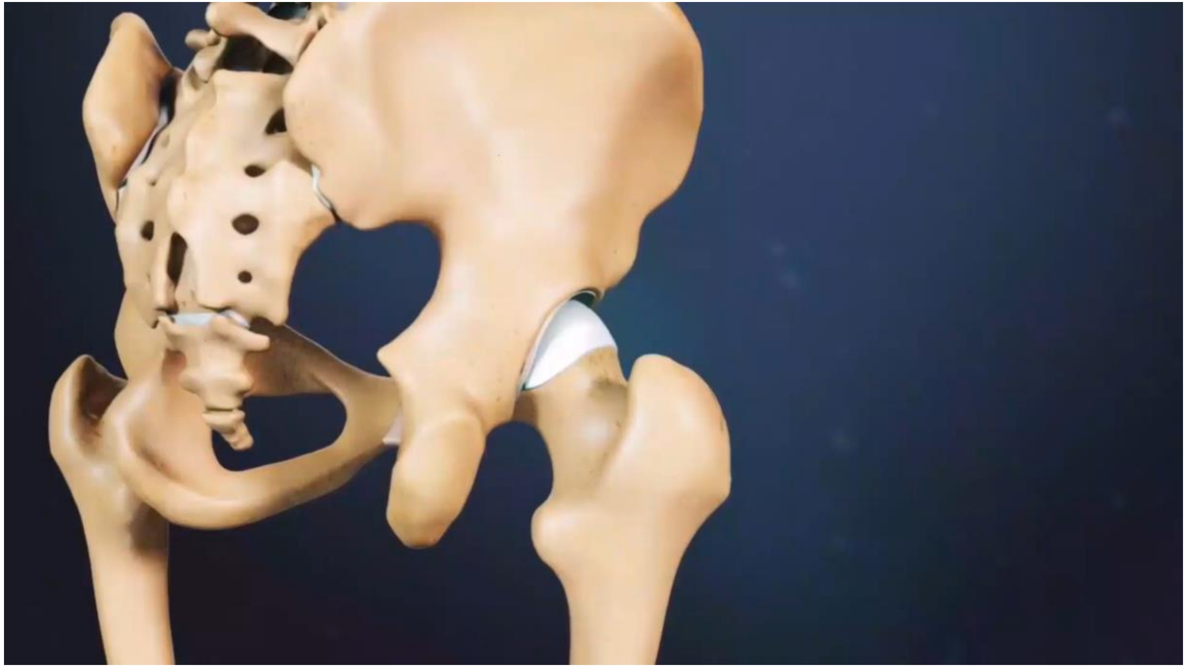
Patient-specific 3D Printed Implants

- Gaining popularity in recent years
- PRosPERoS project
- Design optimization
  - Mechanical stability
  - Biodegradation behavior

Background

- Osteoarthritis
- Hip arthroplasty



(https://www.arthritis-health.com/types/osteoarthritis/videos)

Research Objective

- Goal:

  Tuning the degradation of the implant to the regeneration of the new bone

- Will be achieved by:

  Building a mathematical framework for the assessment of biodegradation

(Source: 3D Systems Inc.)

Model Workflow

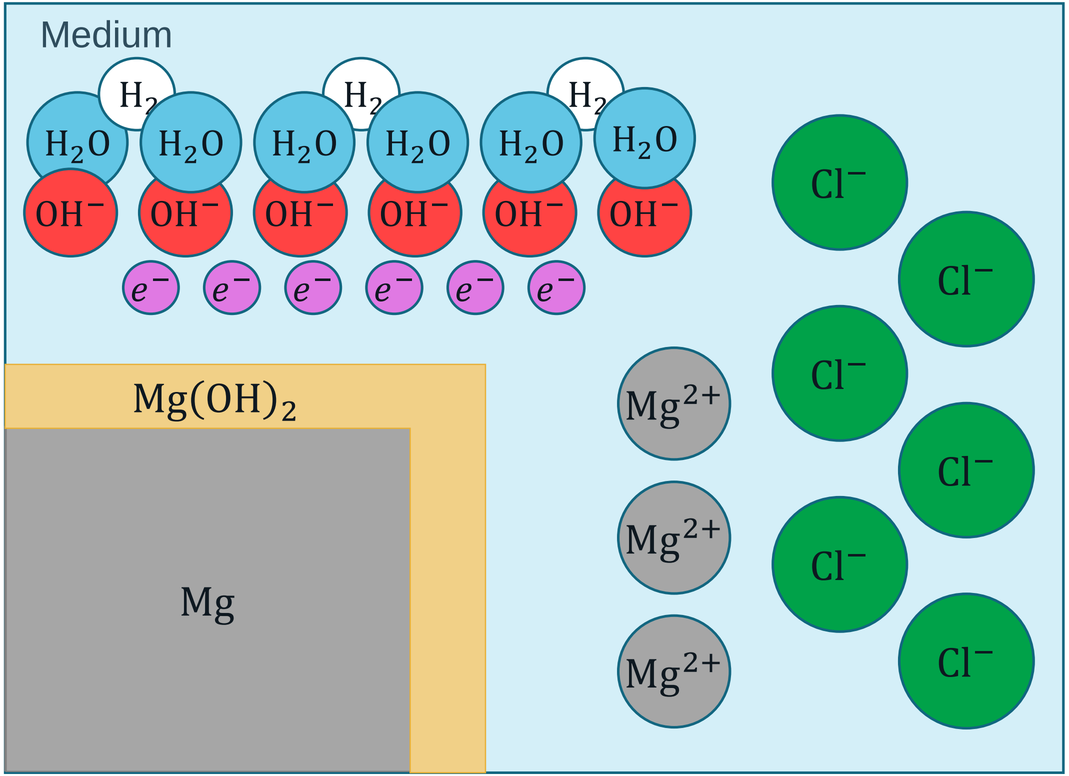
Underlying Science → **Mathematical Models** → **Computational Models**

Underlying Science
- Chemistry of Biodegradation

Mathematical Models
- Partial differential equations
- Reaction-Diffusion-Convection
- Level set method

Computational Models
- Finite difference method
- Finite element method
- Scientific computing libraries
- Open source solvers

Chemistry of Biodegradation



$$Mg \rightarrow Mg^{2+} + 2e^-$$

$$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$$

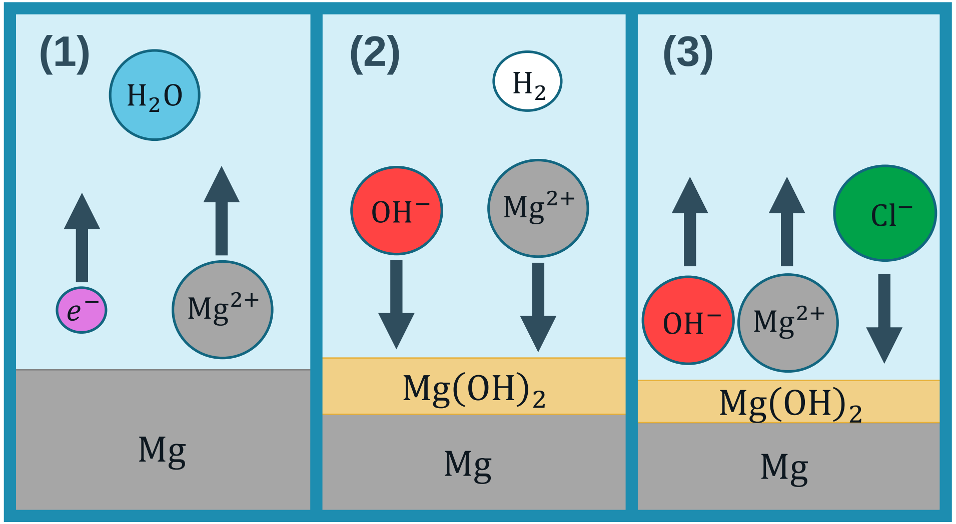
$$Mg^{2+} + 2OH^- \rightarrow Mg(OH)_2$$

$$Mg(OH)_2 + 2Cl^- \rightarrow Mg(Cl)_2 + 2OH^- \rightarrow Mg^{2+} + 2Cl^- + 2OH^-$$

Constructing Mathematical Model

The model captures:

1. The chemistry of dissolution of metallic implant
2. Formation of a protective film
3. Effect of ions in the medium



Mathematical Representation

Chemical reactions

$$Mg + 2H_2O \xrightarrow{k_1} Mg^{2+} + H_2 + 2OH^- \xrightarrow{k_1} Mg(OH)_2 + H_2$$

$$Mg(OH)_2 + 2Cl^- \xrightarrow{k_2} Mg^{2+} + 2Cl^- + 2OH^-$$

Concentration notations

$$Mg^{2+} \rightrightarrows [Mg] \qquad Cl^- \rightrightarrows [Cl]$$

$$Mg(OH)_2 \rightrightarrows F$$

Derived PDEs

$$\frac{\partial [Mg]}{\partial t} = \nabla . \left(D_{Mg}^{e} \nabla [Mg]\right) - k_1 [Mg]\left(1 - \frac{F}{F_{\max}}\right) + k_2 F [Cl]^2$$

$$\frac{\partial F}{\partial t} = k_1 [Mg]\left(1 - \frac{F}{F_{\max}}\right) - k_2 F [Cl]^2$$

$$\frac{\partial [Cl]}{\partial t} = \nabla . \left(D_{Cl}^{e} \nabla [Cl]\right)$$

$$\left(F_{\max} = \rho_{Mg(OH)_2} \times (1 - \epsilon)\right)$$

Capturing the Biodegradation Interface

- Different approaches to track the interface
- A PDE to capture the moving implicit surface
- Level set method

$$\frac{\partial \phi}{\partial t} + \underbrace{\vec{V}.\nabla\phi}_{\text{External velocity field}} + \underbrace{\mathrm{v}|\nabla\phi|}_{\text{Normal direction motion}} = \underbrace{b\kappa|\nabla\phi|}_{\text{Curvature-dependent term}}$$

Level set PDE to solve: $$\frac{\partial \phi}{\partial t} - \frac{D_{\mathrm{Mg}}^{e}\nabla_n[\mathrm{Mg}]}{[\mathrm{Mg}]_{\mathrm{sol}} - [\mathrm{Mg}]_{\mathrm{sat}}}|\nabla\phi| = 0$$

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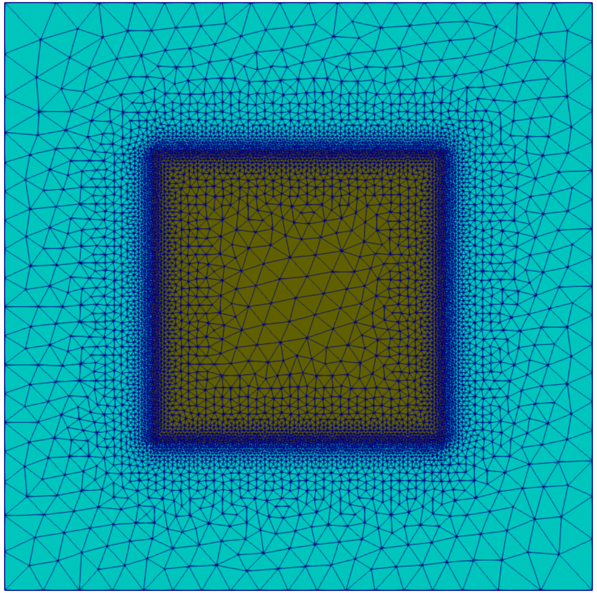
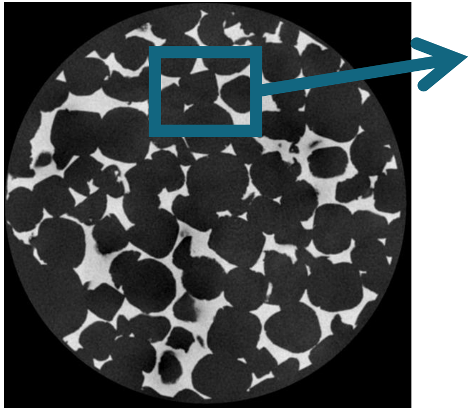
Constructing Computational Model

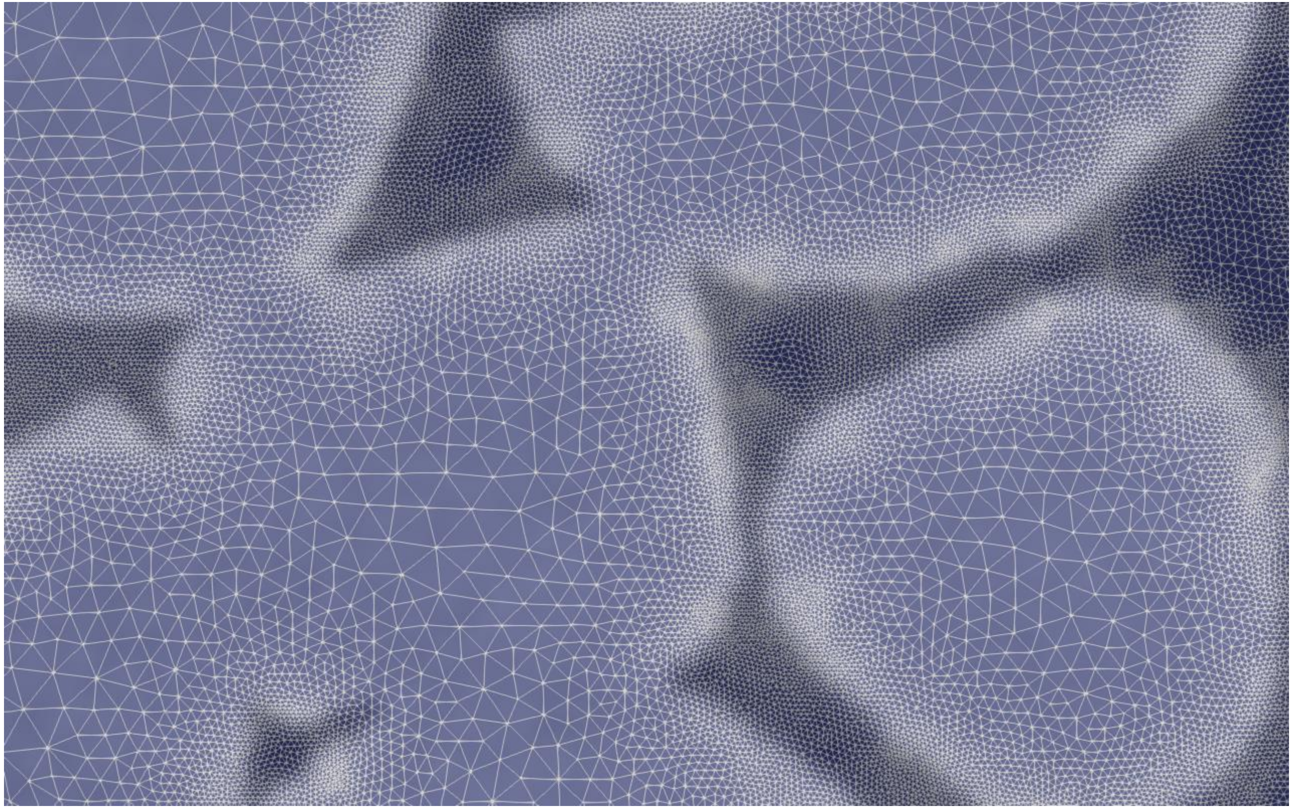
- Not feasible to implement models in sophisticated software packages
- Discretizing PDE equations, numerical computation
  - o Finite difference method (time derivatives)
  - o Finite element method (spatial derivatives)
- Adaptively refined mesh generation



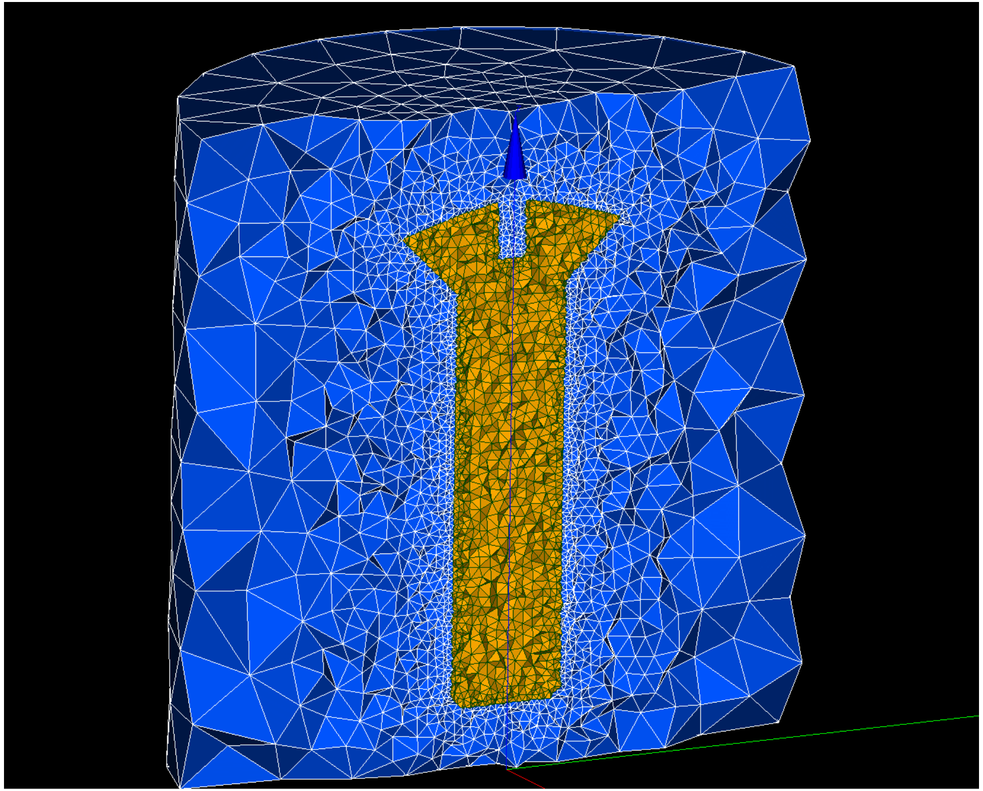
An Example of 2D Mesh

- Sample mesh based on a CT image of a porous Mg scaffold

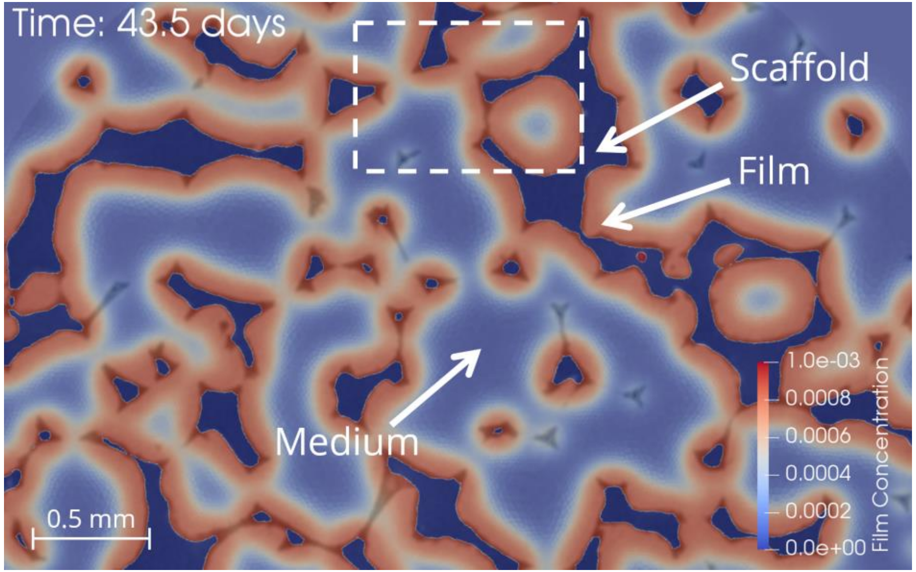


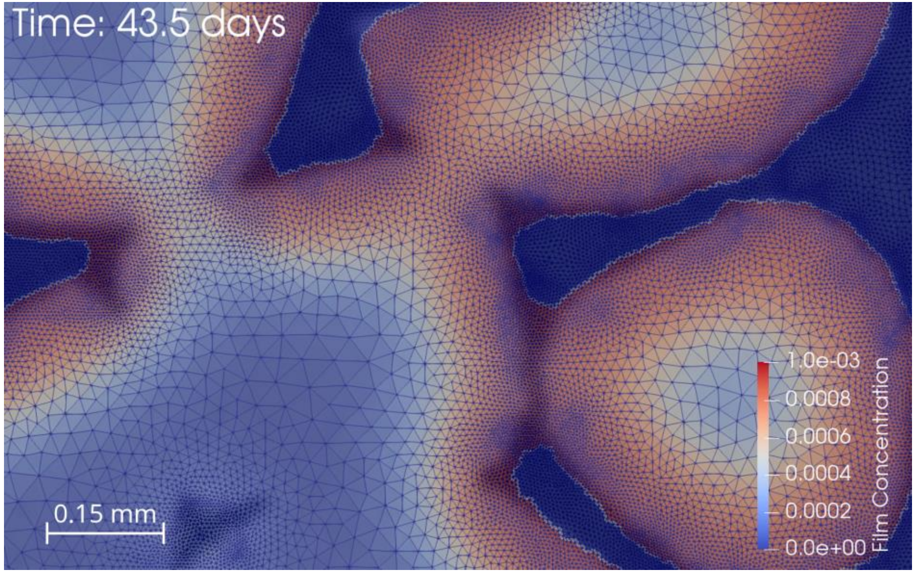


An Example of 3D Mesh

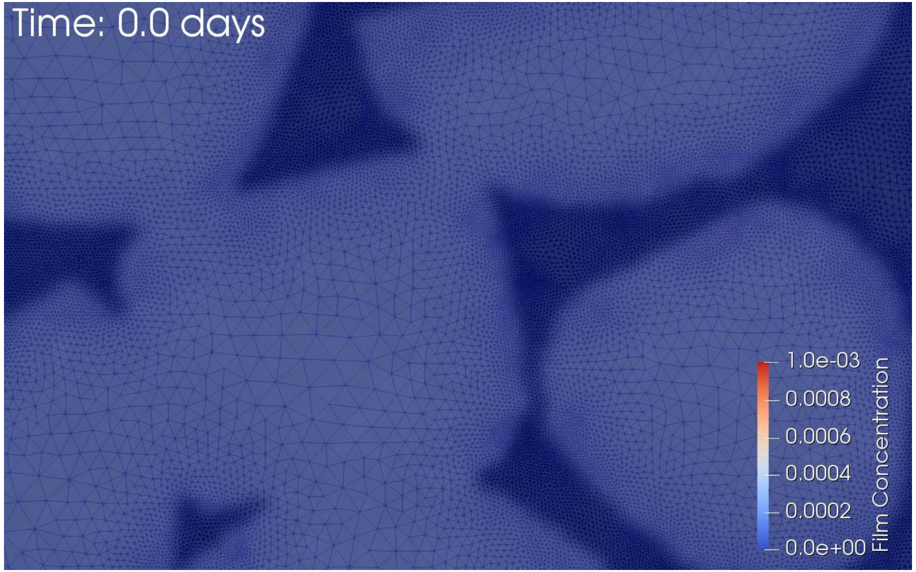


2D Mg Scaffold – Film Formation

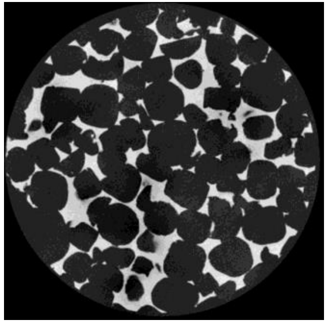




2D Mg Scaffold – Film Formation



2D Mg Scaffold – Film Formation



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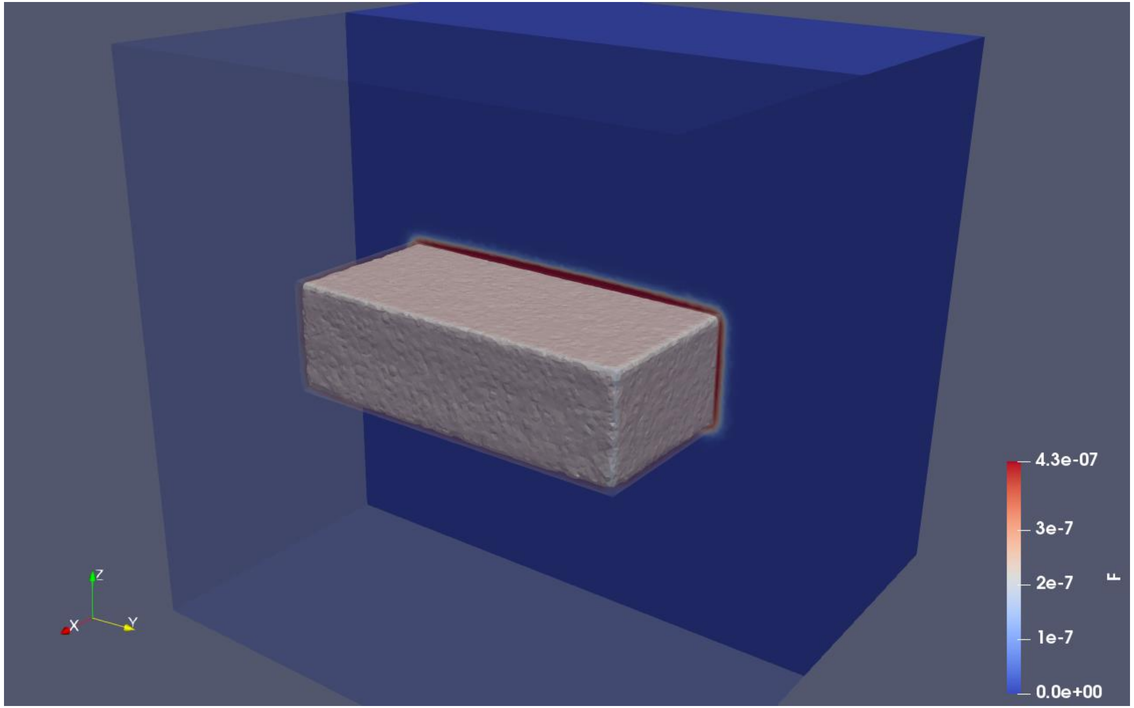
3D Mg Scaffold – Protective Film



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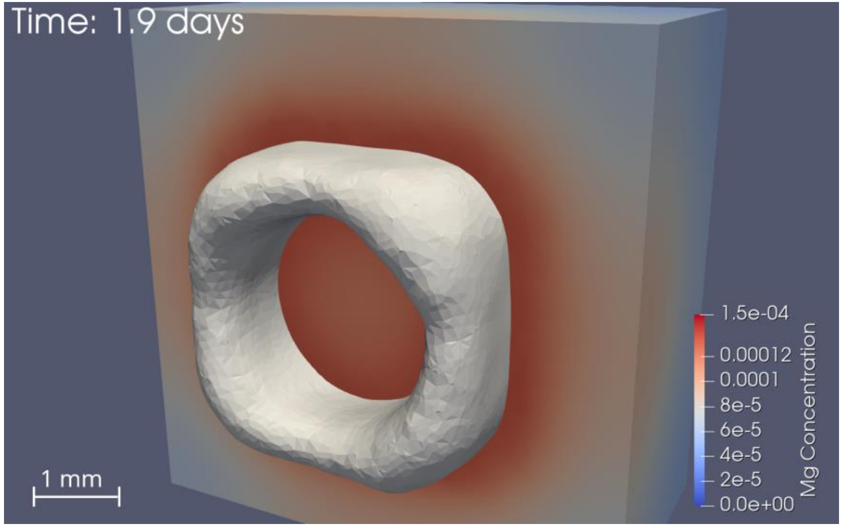
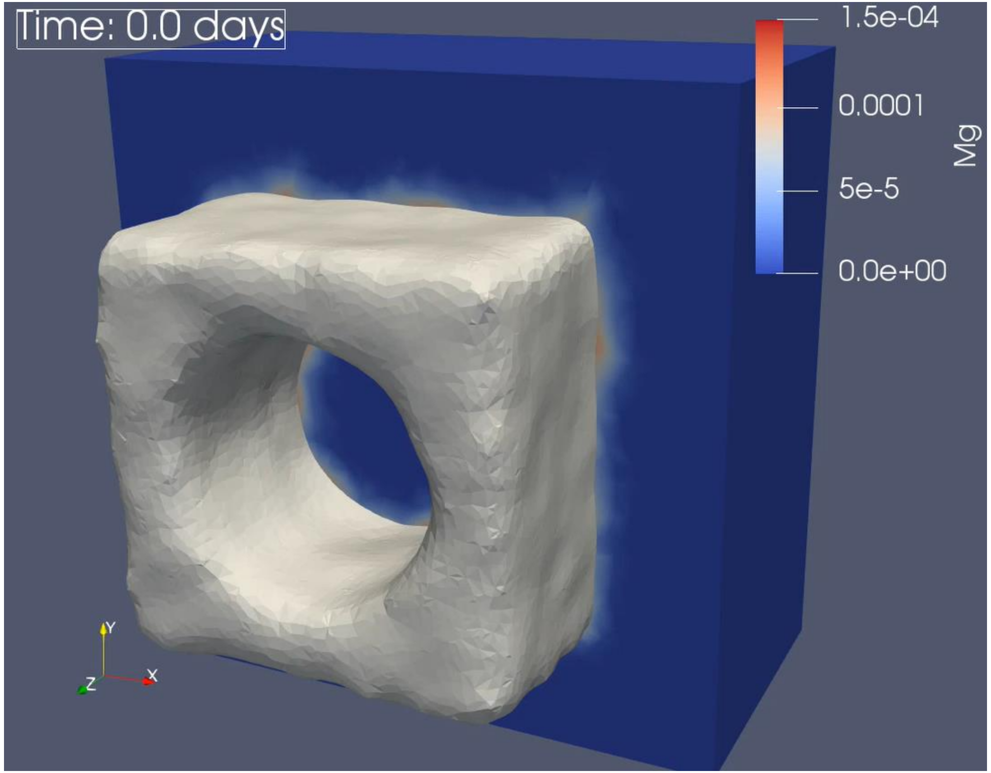
3D Mg Scaffold – Mg^{2+} Release





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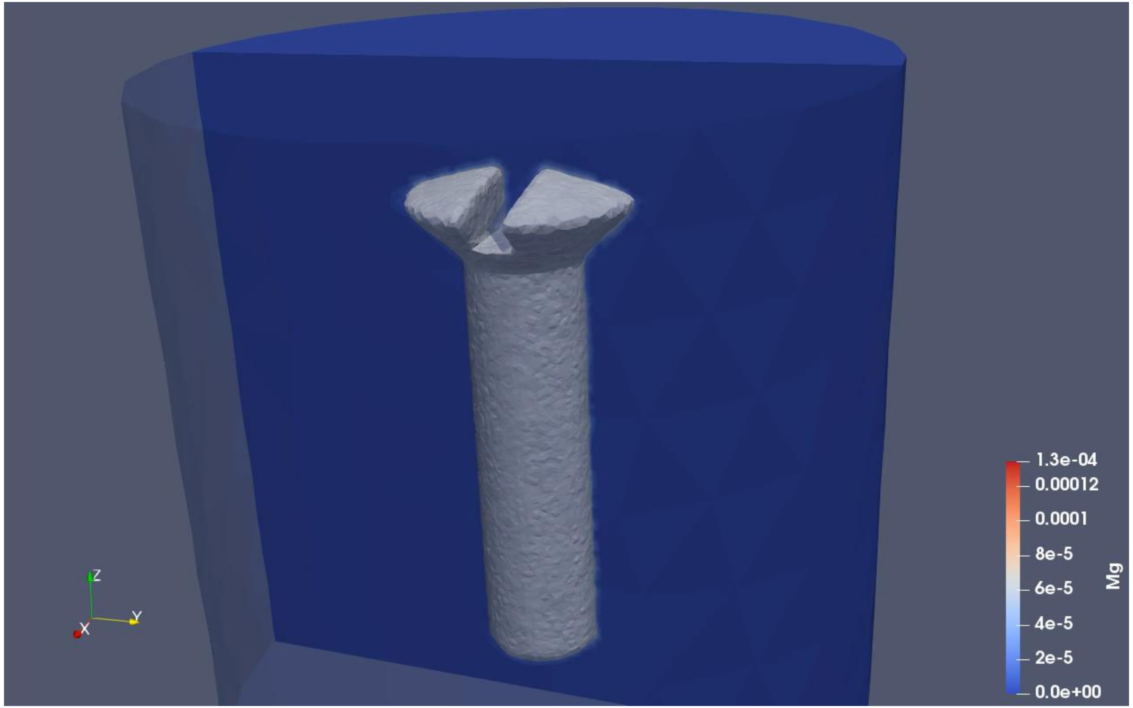
Screw Biodegradation – Ion Release



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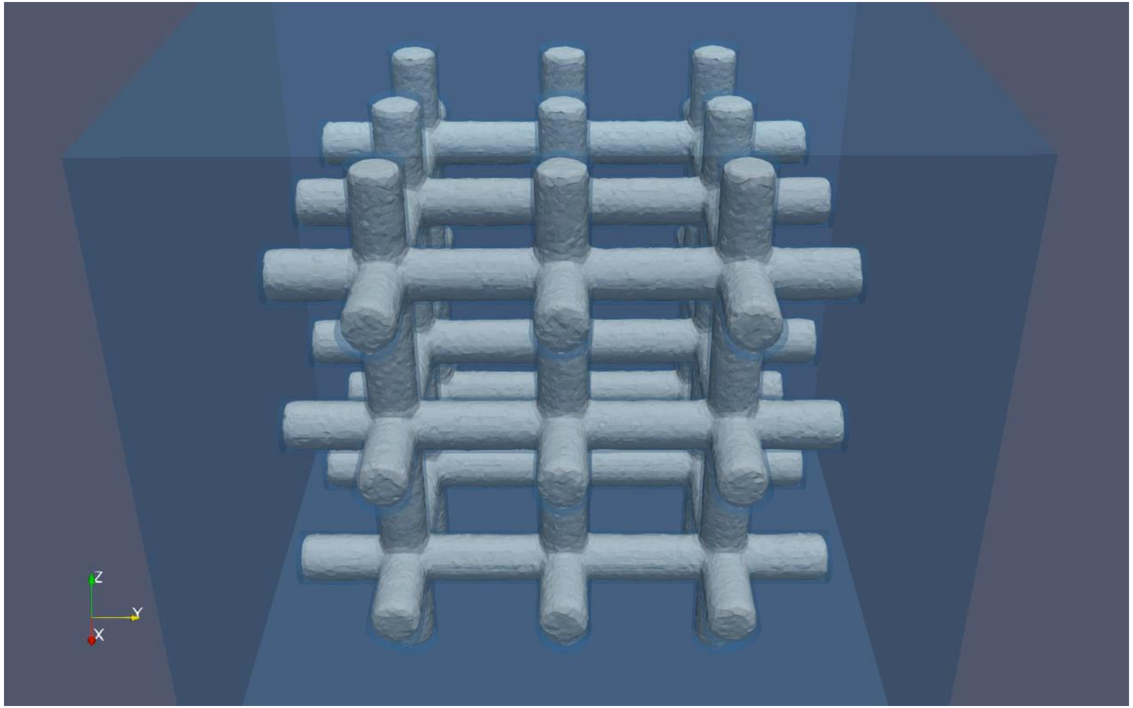
Porous Scaffold Degradation



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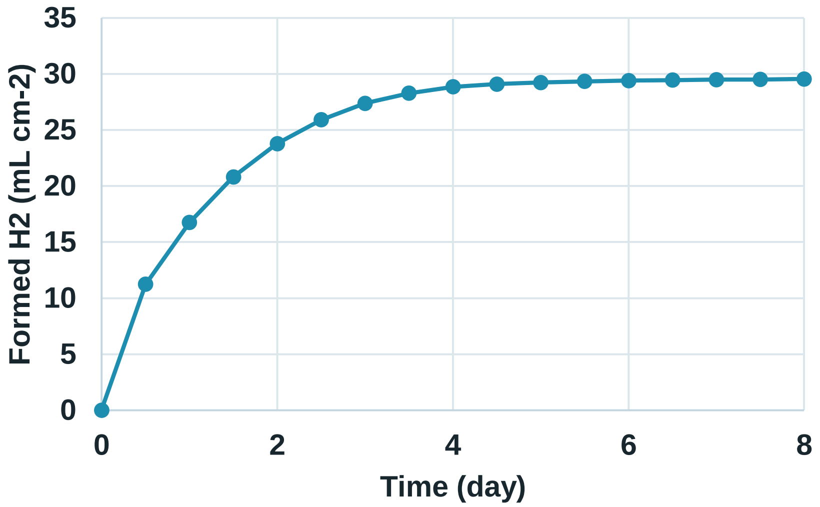
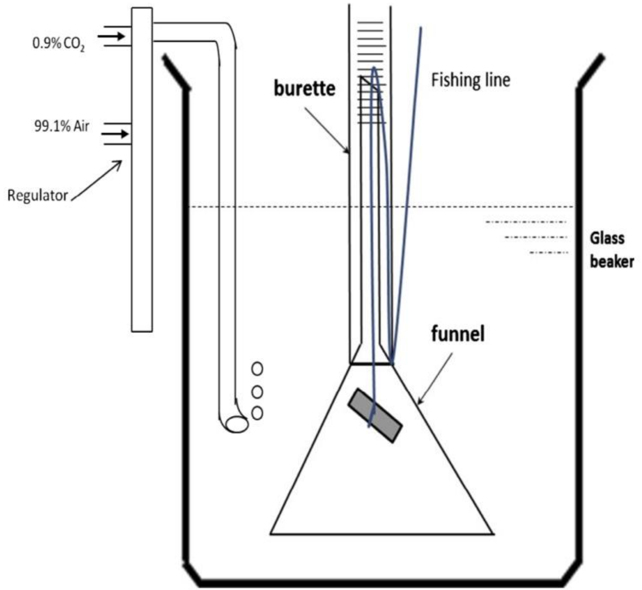
Verification and Validation

- Different bioreactor setups for in-vitro data
- Different approaches to validate models
  - Mass loss
  - Hydrogen evolution
- Sensitivity analysis and convergence studies

Static Experimental Setup

- Immersion tests for sample scaffolds
- Measuring formed hydrogen gas





(Abidin et al., Corrosion Science, 2013)

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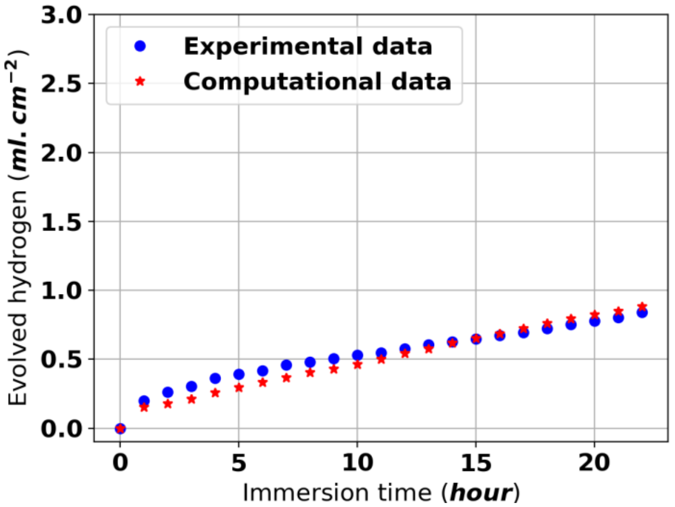
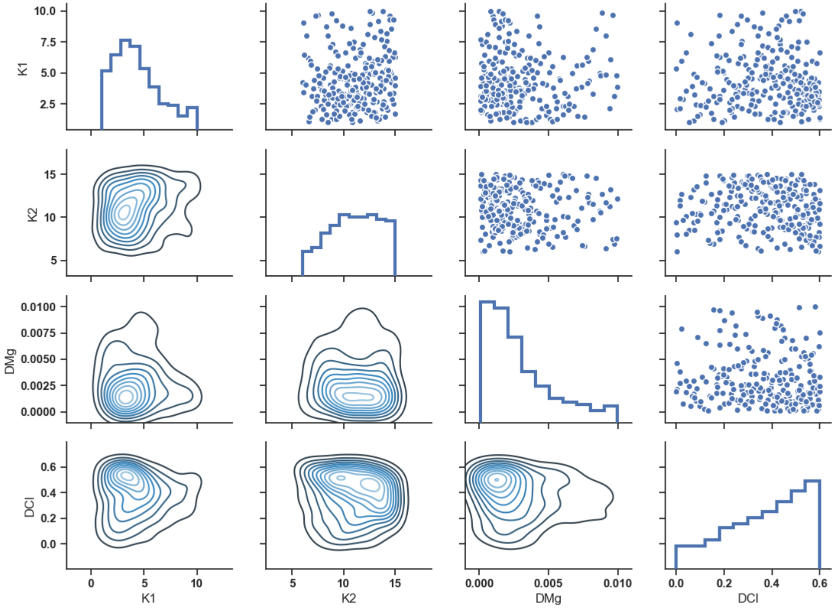
Model Calibration and Parameter Estimation

- Estimating reaction rates and diffusion coefficients
- Using a Bayesian optimization algorithm





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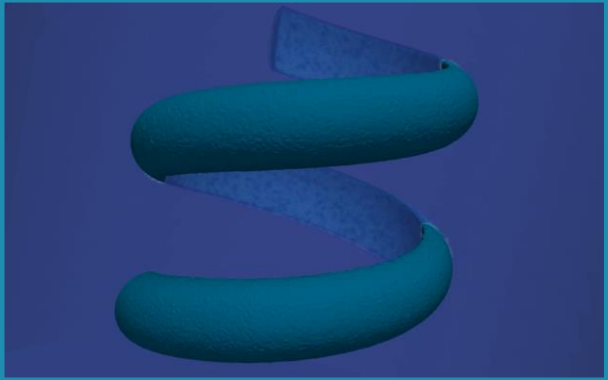
Conclusion

- A quantitative mathematical model to assess the degradation behavior of biodegradable metallic implants in silico
- Once fully validated, the model will be an important tool to find the right design and properties of the magnesium-based implants for specific orthopedic applications



Thank you for your attention

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