

High-Performance Numerical Simulation of Biodegradation Process with Moving Boundaries

FreeFEM Days, 11th Edition

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0 Our Research Group

- ▶ Supervisor: Prof. Ir. Liesbet Geris
- ▶ Research profile:
Computational Tissue Engineering, Computational Biomechanics,
Computational Biology, Computational Genomics



1 Outline

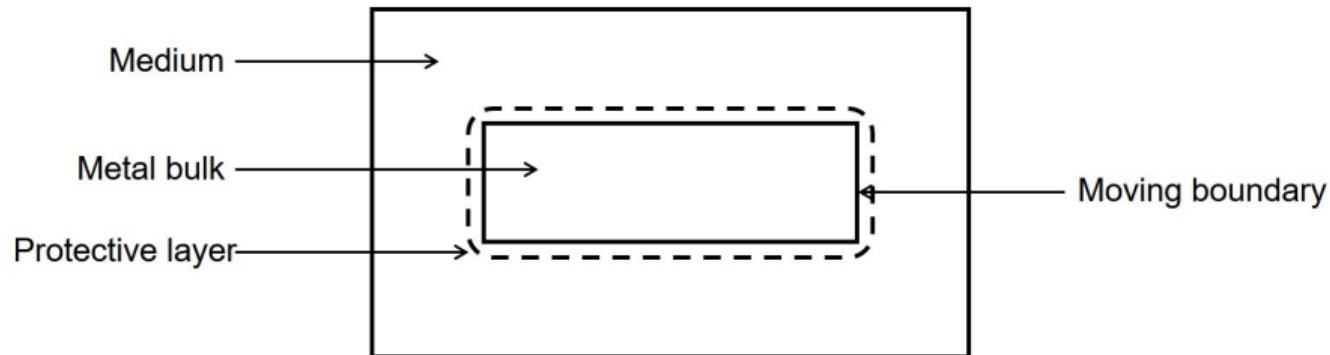
- ① Introduction
- ② Mathematical Model
- ③ Computational Model and Parallelization
- ④ Simulation Results
- ⑤ Performance Analysis

1 Reaction-Diffusion Systems with Moving Boundaries

- ▶ Stefan problems
- ▶ Diffusion-controlled interface
- ▶ Diffusion and reaction lead to the change of domain geometry
- ▶ Degradation is an example of such a system

1 Biodegradation Process

- ▶ Dissolution of the bulk material
- ▶ Formation of a protective film
- ▶ Effect of ions in the medium



1 A Sample Application

- ▶ Hip joint replacement implants
- ▶ Tuning the degradation parameters to the rate of bone growth

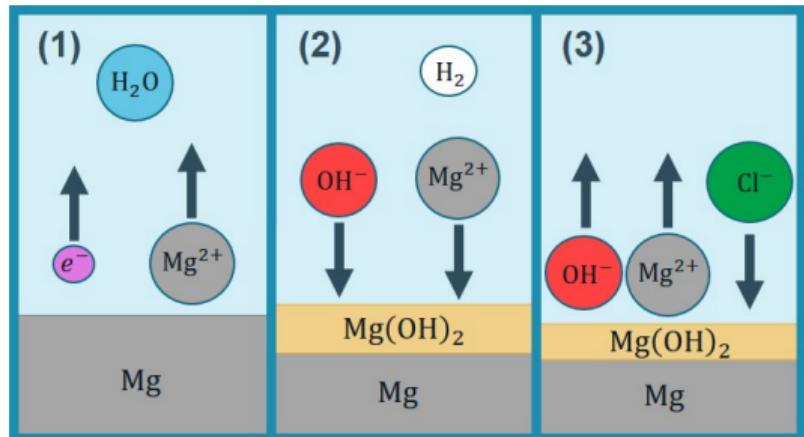
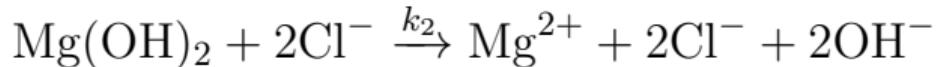
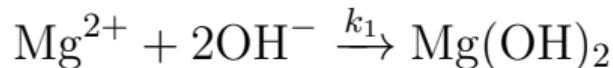
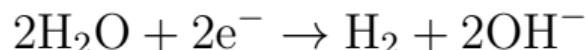
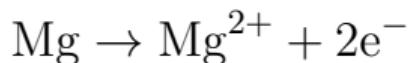


2 Outline

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2 Chemistry of Biodegradation

Some of the chemical reactions:



2 Reaction-Diffusion Equations

$$C_{\text{Mg}} = C_{\text{Mg}}(x, t), \quad C_{\text{Film}} = C_{\text{Film}}(x, t) \quad x \in \Omega \subset \mathbb{R}^3$$

$$\frac{\partial C_{\text{Mg}}}{\partial t} = \nabla \bullet (D_{\text{Mg}}^e \bullet \nabla C_{\text{Mg}}) - k_1 C_{\text{Mg}} \left(1 - \frac{C_{\text{Film}}}{[\text{Film}]_{\max}} \right) + k_2 C_{\text{Film}} [\text{Cl}]^2$$

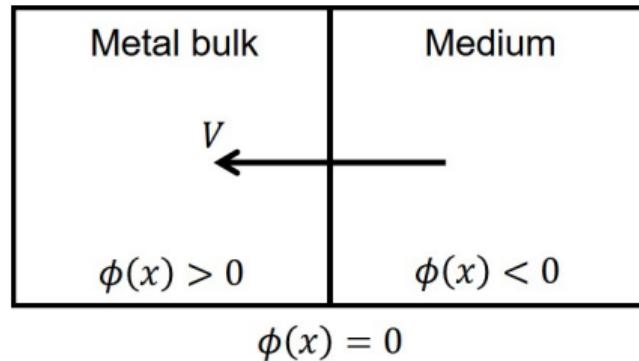
$$\frac{\partial C_{\text{Film}}}{\partial t} = k_1 C_{\text{Mg}} \left(1 - \frac{C_{\text{Film}}}{[\text{Film}]_{\max}} \right) - k_2 C_{\text{Film}} [\text{Cl}]^2$$

$$D_{\text{Mg}}^e = D_{\text{Mg}} \left(\left(1 - \frac{C_{\text{Film}}}{[\text{Film}]_{\max}} \right) + \frac{C_{\text{Film}}}{[\text{Film}]_{\max}} \frac{\epsilon}{\tau} \right)$$

2 Level Set Method

Implicit signed distance function $\phi = \phi(x, t)$ $x \in \Omega \subset \mathbb{R}^3$

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



2 Coupling Mass Transfer and Level Set

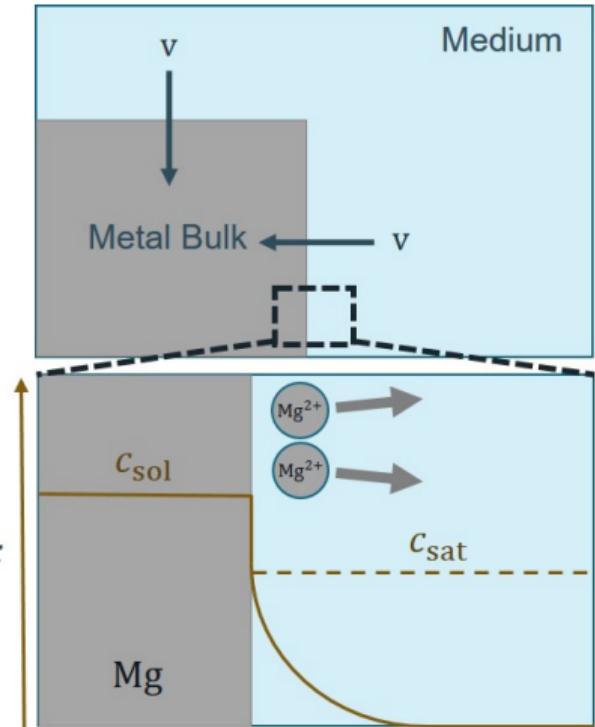
$$\frac{\partial \phi}{\partial t} + v |\nabla \phi| = 0$$

Rankine-Hugoniot:

$$\{ \mathbf{J}(x, t) - (c_{\text{sol}} - c_{\text{sat}}) \mathbf{v}(x, t) \} \cdot \mathbf{n} = 0$$

$$D_{\text{Mg}}^e \nabla_n C_{\text{Mg}} - ([\text{Mg}]_{\text{sol}} - [\text{Mg}]_{\text{sat}}) \mathbf{v} = 0$$

$$\frac{\partial \phi}{\partial t} - \frac{D_{\text{Mg}}^e \nabla_n C_{\text{Mg}}}{[\text{Mg}]_{\text{sol}} - [\text{Mg}]_{\text{sat}}} |\nabla \phi| = 0$$



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3 Weak Formulation

Rewriting the diffusion-reaction PDE:

$$\frac{\partial u}{\partial t} = \nabla \bullet (D \bullet \nabla u) - k_1 bu + k_2 pq^2$$

Defining trial and test function space:

$$\mathcal{S}_t = \left\{ u(\mathbf{x}, t) \mid \mathbf{x} \in \Omega, t > 0, u(\mathbf{x}, t) \in \mathcal{H}^1(\Omega), \text{ and } \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma \right\}$$

$$\mathcal{V} = \left\{ v(\mathbf{x}) \mid \mathbf{x} \in \Omega, v(\mathbf{x}) \in \mathcal{H}^1(\Omega), \text{ and } v(\mathbf{x}) = 0 \text{ on } \Gamma \right\}$$

3 Weak Formulation cont.

$$\frac{\partial u}{\partial t}v = \nabla \bullet (D \bullet \nabla u)v - k_1bu v + k_2pq^2v \quad \forall v \in \mathcal{V}$$

Integrate over the whole domain:

$$\int_{\Omega} \frac{\partial u}{\partial t}vd\omega = \int_{\Omega} \nabla \bullet (D \bullet \nabla u)vd\omega - \int_{\Omega} k_1bu v d\omega + \int_{\Omega} k_2pq^2v d\omega$$

Integration by part, Green's divergence theory, Backward Euler scheme:

$$\int_{\Omega} \frac{u - u^n}{\Delta t}vd\omega = \int_{\Gamma} Dv \bullet \frac{\partial u}{\partial n}d\gamma - \int_{\Omega} D \bullet \nabla u \bullet \nabla v d\omega - \int_{\Omega} k_1bu v d\omega + \int_{\Omega} k_2pq^2v d\omega$$

3 Weak Formulation cont.

$$\int_{\Omega} uv d\omega + \int_{\Omega} \Delta t D \bullet \nabla \bullet u \nabla v d\omega + \int_{\Omega} \Delta t k_1 b u v d\omega = \int_{\Omega} u^n v d\omega + \int_{\Omega} \Delta t k_2 p q^2 v d\omega$$

By defining a linear functional $(f, v) = \int_{\Omega} f v d\omega$

$$(u, v)[1 + \Delta t k_1 b] + \Delta t(D \nabla u, \nabla v) = (u^n, v) + \Delta t(f^n, v)$$

multiplying to a new coefficient $\alpha = \frac{1}{1 + \Delta t k_1 b}$

$$(u, v) + \alpha \Delta t(D \nabla u, \nabla v) = \alpha(u^n, v) + \alpha \Delta t(f^n, v)$$

3 Discretization Scheme

$$\mathcal{V}_h = \text{span} \left(\{\psi_i\}_{i \in \mathcal{I}_s} \right) \quad \mathcal{I}_s = \{0, \dots, N\}$$

Using 1st order Lagrange polynomials as basis functions

$$u = \sum_{j=0}^N c_j \psi_j(\boldsymbol{x}), \quad u^n = \sum_{j=0}^N c_j^n \psi_j(\boldsymbol{x})$$

$$\sum_{j=0}^N (\psi_i, \psi_j) c_j + \alpha \Delta t \sum_{j=0}^N (\nabla \psi_i, D \nabla \psi_j) c_j = \sum_{j=0}^N (\psi_i, \psi_j) c_j^n + \Delta t (f^n, \psi_i)$$

3 Discretization Scheme cont.

A linear system of equations

$$\sum_j A_{i,j} c_j = b_i$$

$$A_{i,j} = (\psi_i, \psi_j) + \alpha \Delta t (\nabla \psi_i, D \nabla \psi_j)$$

$$b_i = \sum_{j=0}^N \alpha (\psi_i, \psi_j) c_j^n + \alpha \Delta t (f^n, \psi_i)$$

3 Discretization Scheme cont.

Final form as implemented in FreeFEM

$$(M + \alpha \Delta t K) c = \alpha M c_1 + \alpha \Delta t f$$

$$M = \{M_{i,j}\}, \quad M_{i,j} = (\psi_i, \psi_j), \quad i, j \in \mathcal{I}_s$$

$$K = \{K_{i,j}\}, \quad K_{i,j} = (\nabla \psi_i, D \nabla \psi_j), \quad i, j \in \mathcal{I}_s$$

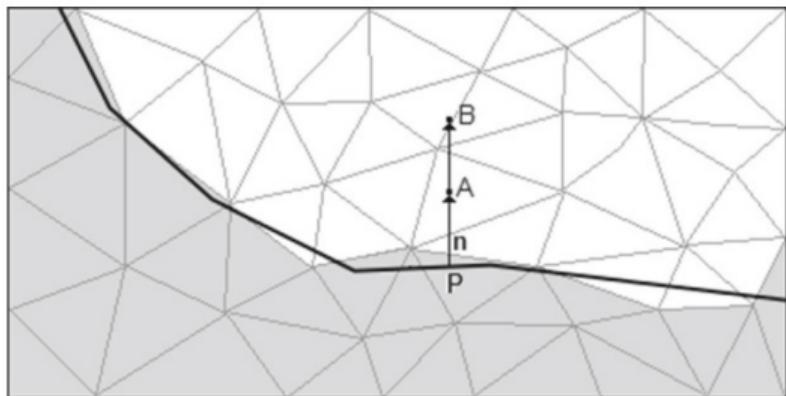
$$f = \{f_i\}, \quad f_i = (f(\mathbf{x}, t_n), \psi_i), \quad i \in \mathcal{I}_s$$

$$c = \{c_i\}, \quad i \in \mathcal{I}_s$$

$$c_1 = \{c_i^n\}, \quad i \in \mathcal{I}_s$$

3 Level Set Implementation

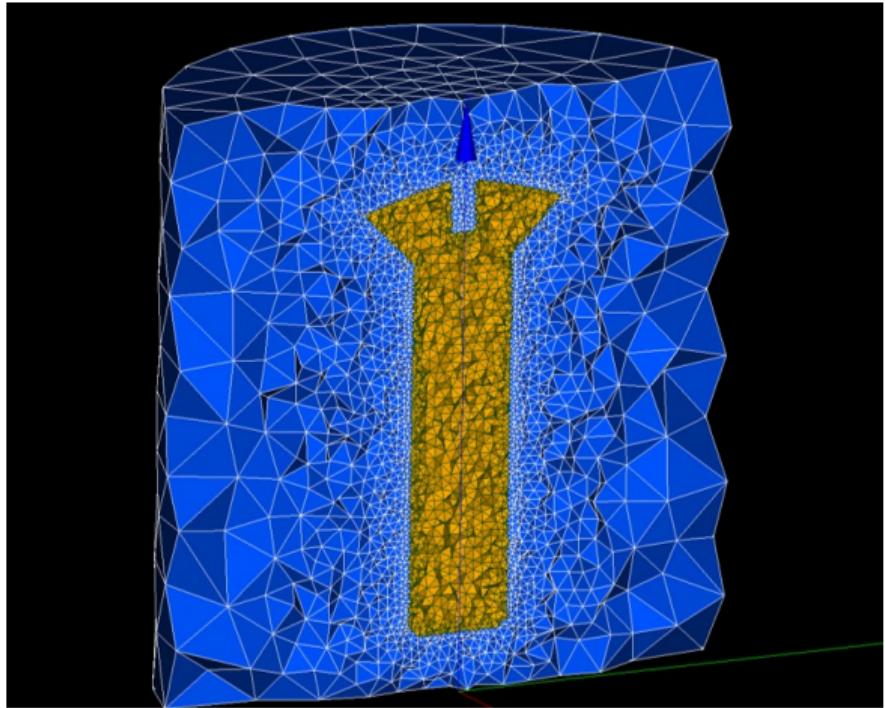
- ▶ Penalization for interface BCs
- ▶ Computing $\nabla_n C_{\text{Mg}}$ correctly
- ▶ Problem of oscillation
- ▶ Too flat or too steep gradients
- ▶ Nightmare of re-distancing



(P. Bajger et al. 2017)

3 Computational Mesh

- ▶ Eulerian mesh
- ▶ Generated using Netgen in SALOME platform
- ▶ Adaptively refined on the moving interface



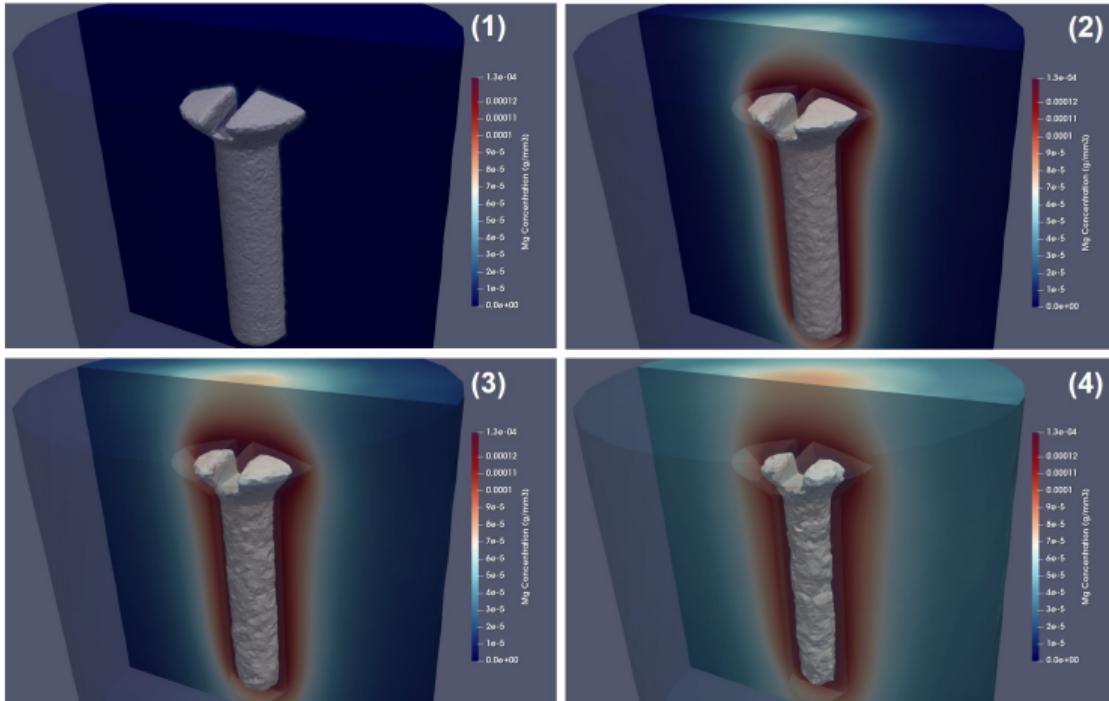
3 Parallelization

- ▶ Message Passing Interface
- ▶ Distributed numerical integration
(assigning a number in the range of [0, MPI Size-1] to each element)
- ▶ MUMPS multifrontal direct solver

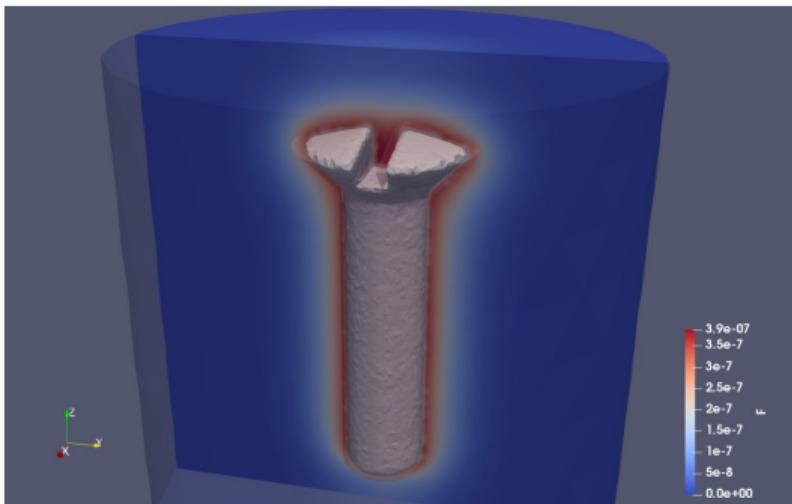
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4 Release of Ions and Degradation - Simple Screw

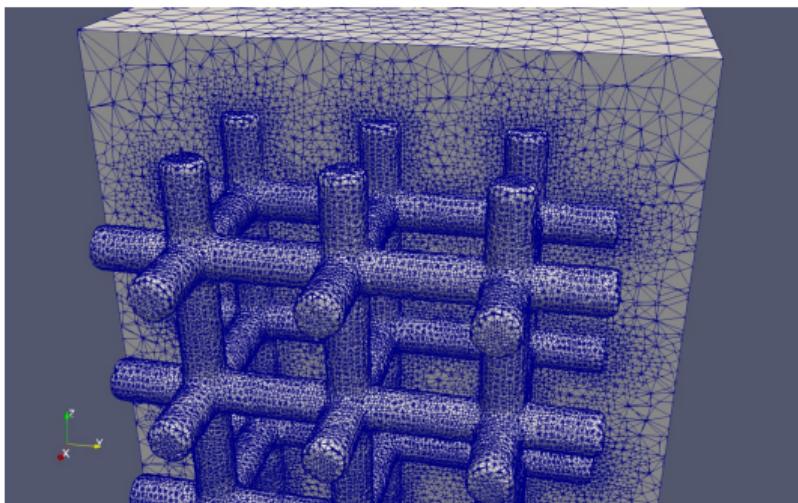


4 Film Formation - Simple Screw

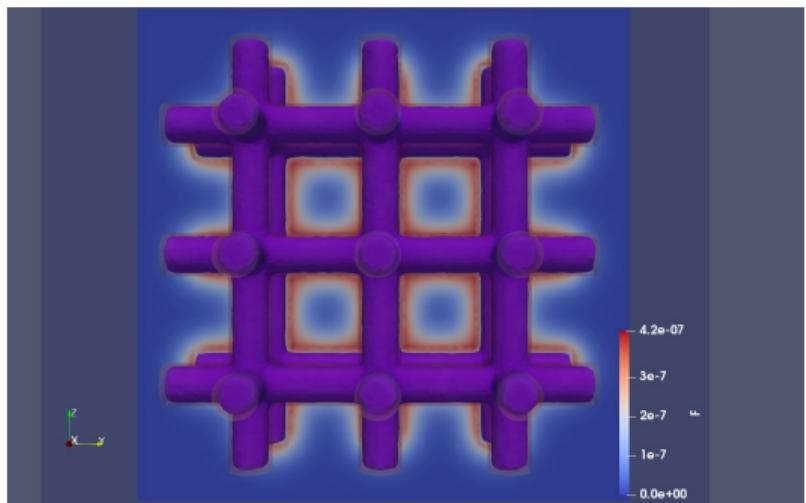


Formation of the protective film on the interface of material-medium

4 Release of Ions and Degradation - Porous Structure



Trimmed view of the computational mesh



Formation of the protective film

4 Quantitative Results

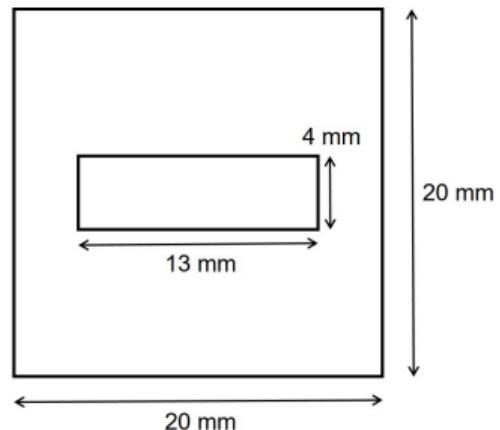
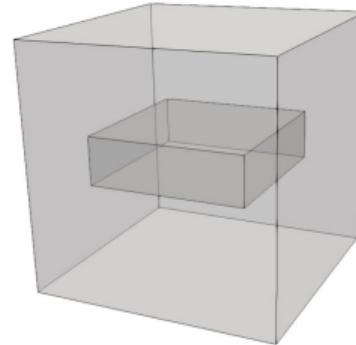
Measuring mass loss:

- ▶ Direct weight reduction
- ▶ Side products evolution

Using level set output for calculating mass loss

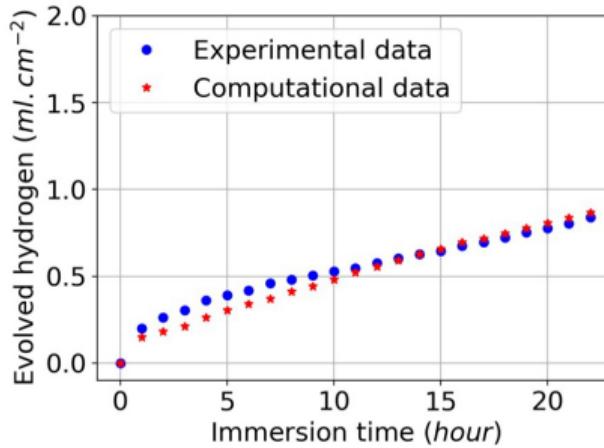
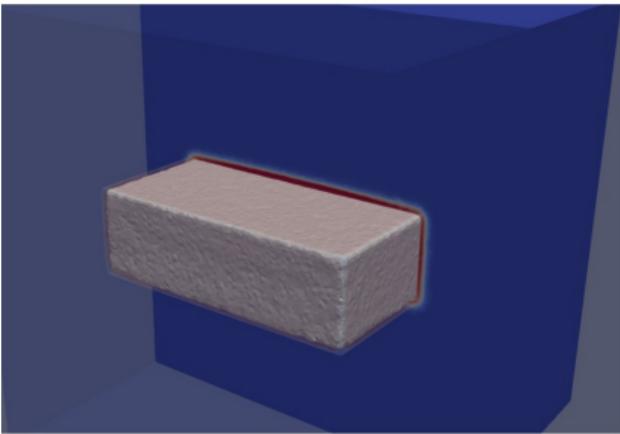
$$Mg_{\text{lost}} = \int_{\Omega_+(t)} Mg_{\text{solid}} dV - \int_{\Omega_+(0)} Mg_{\text{solid}} dV_0$$

$$\Omega_+(t) = \{\mathbf{x} : \phi(\mathbf{x}, t) \geq 0\}$$



Simulation and experimental setup

4 Mass Loss and Evolving Side Products



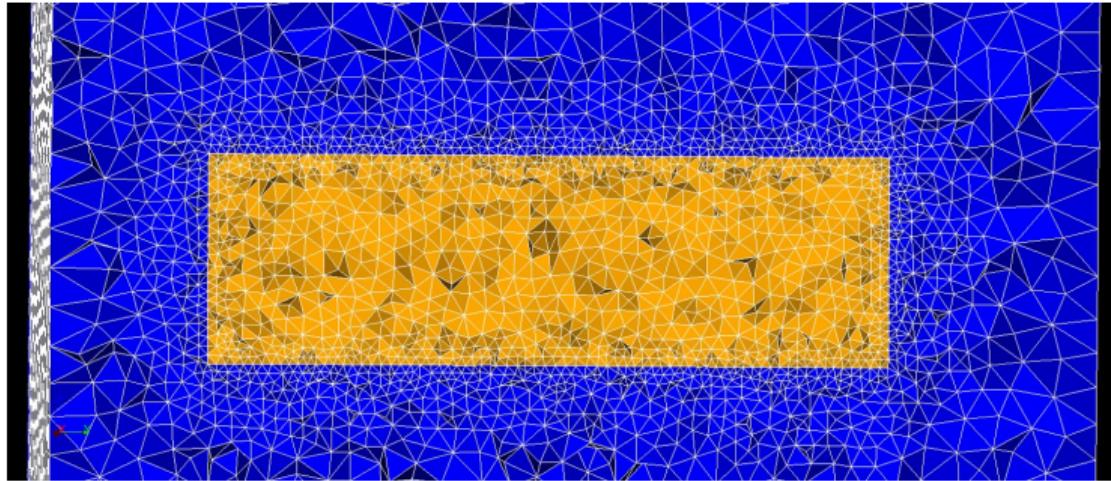
Film formation and the comparison of predicted and experimental mass loss, measured by the evolved hydrogen gas

5 Outline

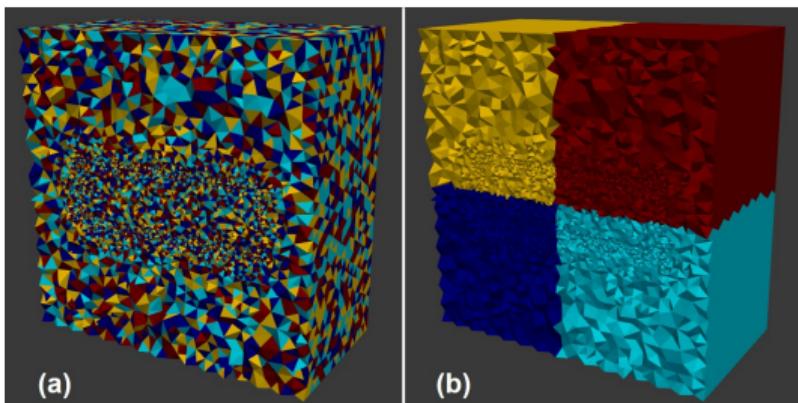
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5 Problem Size

- ▶ Same setup as the model for calibration and validation
- ▶ DOF: 144k
- ▶ Elements: 831k (P1)



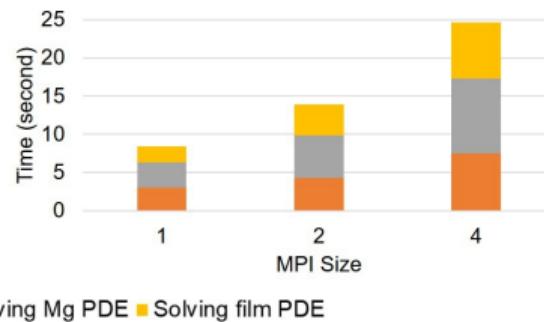
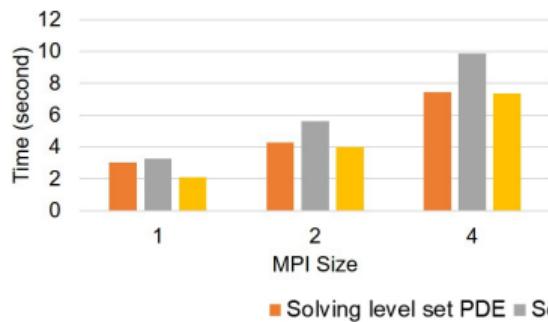
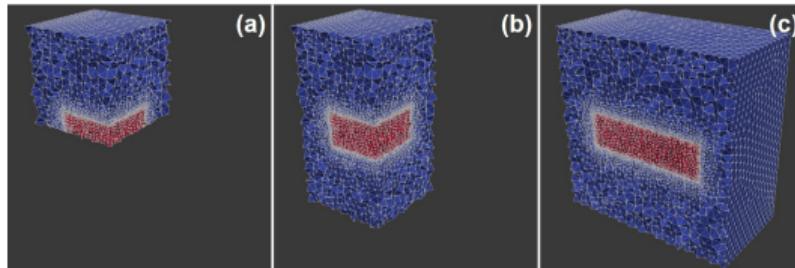
5 Domain Decomposition



Two different approaches for domain decomposition.
Colors show different mesh regions assigned to
different MPI cores.



5 Weak-Scaling Test Results

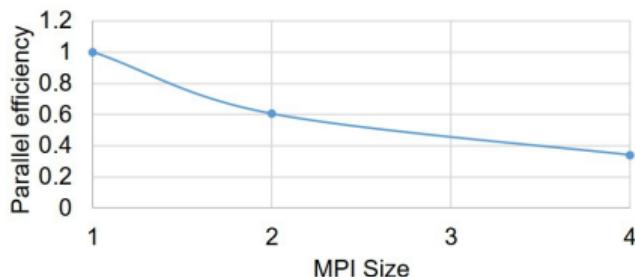
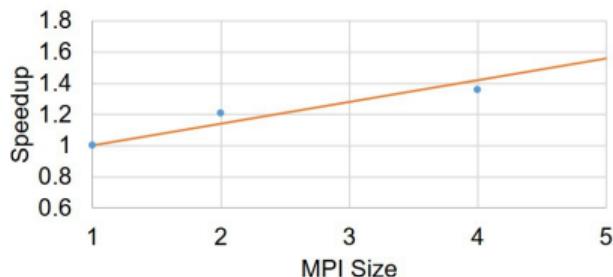


5 Weak-Scaling Test Analysis

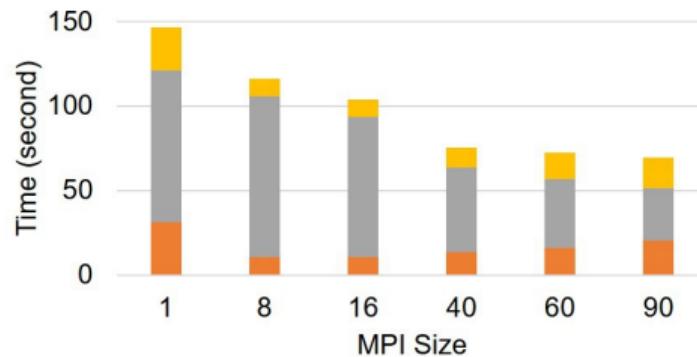
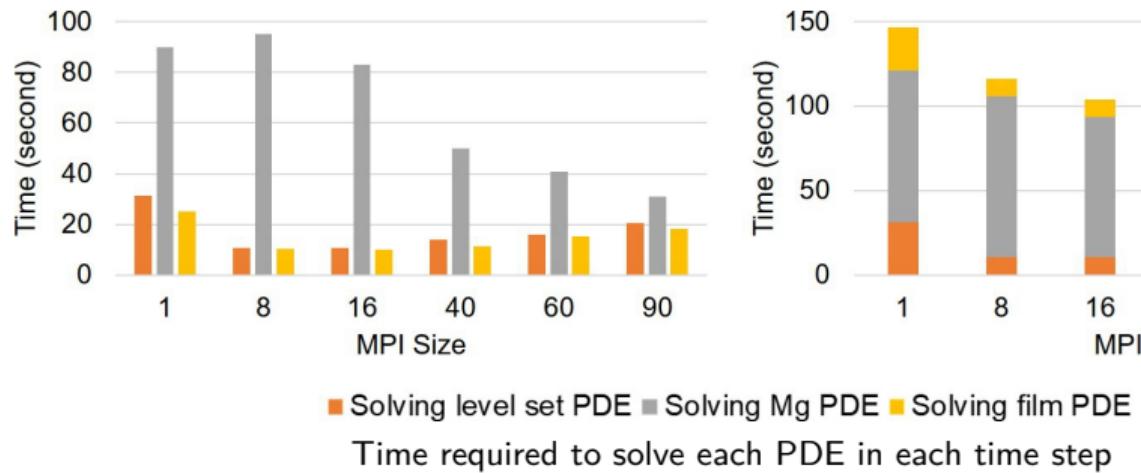
Based on Gustafson's law:

$$\text{Speedup} = f + (1 - f) \times N$$

Serial proportion = 86%, Parallelizable proportion = 14%



5 Strong-Scaling Test Results

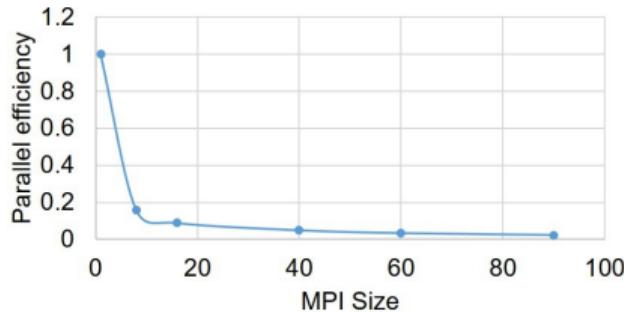
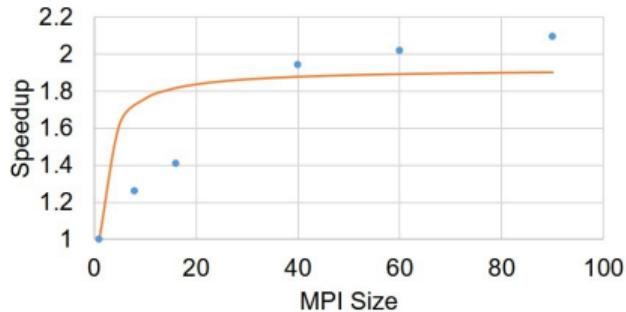


5 Strong-Scaling Test Analysis

Based on Amdahl's law:

$$\text{Speedup} = \frac{1}{f + \frac{1-f}{N}}$$

Serial proportion = 52%, Parallelizable proportion = 48%



5 Conclusion

- ▶ A quantitative mathematical model and its corresponding computational model to assess the degradation behavior of biodegradable materials
- ▶ Using level set method to track the moving corrosion front during degradation
- ▶ Once fully validated, the model will be an important tool to find the right design and properties of the metallic biomaterials and implants

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