Mathematical investigation of corrosion behavior of bioabsorbable metals on the biodegradation interface

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Statement of Need
& Basic Concepts

Biodegradable Metals

- Mg, Zn, and Fe
- Gradually disappear/absorbed and replaced by new tissue/bone
- Great mechanical/biological properties
- The controlled release profile is an issue for different types of implants
- The degradation behavior should be tuned/optimized for various applications

(Han et al., Mater. Today, 23, 2019)

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Problem Definition

- Challenge:
  - Tuning the biodegradation to the regeneration of the new tissue/bone
  - Optimizing the implant design based on the release profile
- Can be solved by:
  - Mathematical modeling of biodegradation
  - Coupling biodegradation models with tissue growth models
  - Considering environmental effects

Modeling Workflow

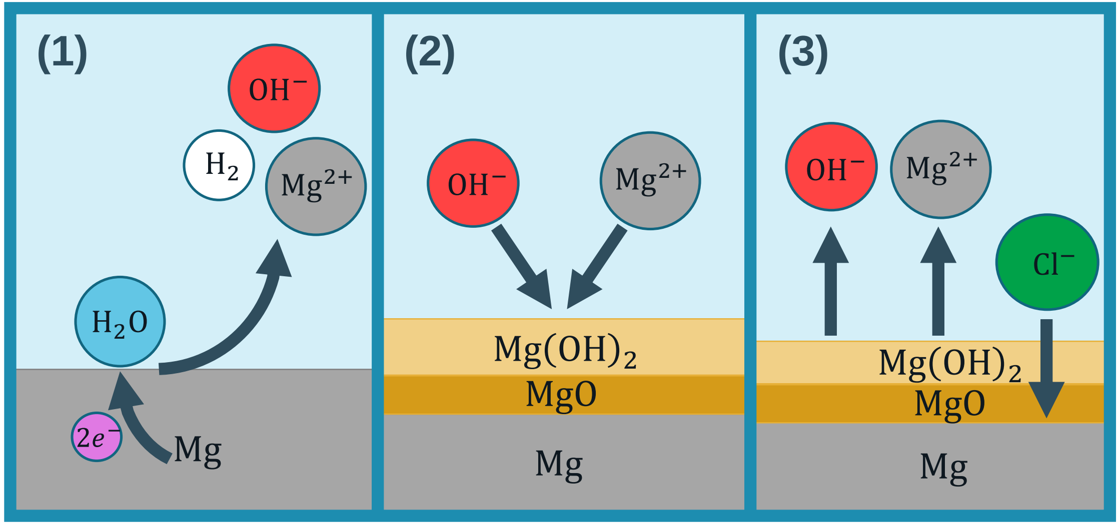
Underlying Science	**Mathematical Models**	**Computational Models**
Chemistry of biodegradation	Partial differential equations	Finite element method
Physics of perfusion	Reaction-Diffusion-Convection	Finite difference method
Biology of tissue growth	Navier-Stokes equations	Parallel computing libraries
	Level-set / Phase-field	Open source solvers

Biodegradation Framework

Chemistry of Biodegradation

The model captures:

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



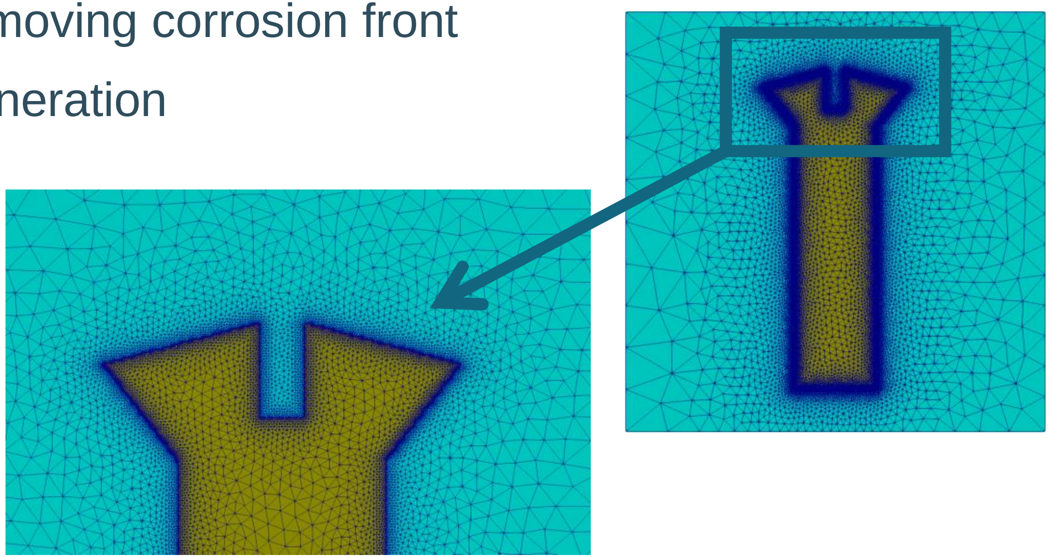
Constructing Mathematical Model

- Converting the chemical interaction into mathematical forms
- Reaction-diffusion-convection partial differential equations (PDE)
- An example for the transport of Mg ions

$$\frac{\partial C_{\mathrm{Mg}}}{\partial t} = \underbrace{\nabla.\left(D_{\mathrm{Mg}}^{e} \nabla C_{\mathrm{Mg}}\right)}_{\text{Diffusion}} - \underbrace{\nabla.\left(\mathrm{v} C_{\mathrm{Mg}}\right)}_{\text{Convection}} \underbrace{- k_1 C_{\mathrm{Mg}} \left(1 - \beta \frac{C_{\mathrm{Film}}}{[\mathrm{Film}]_{\mathrm{max}}}\right) + k_2 C_{\mathrm{Film}} {C_{\mathrm{Cl}}}^2}_{\text{Reaction}}$$

Constructing Computational Model

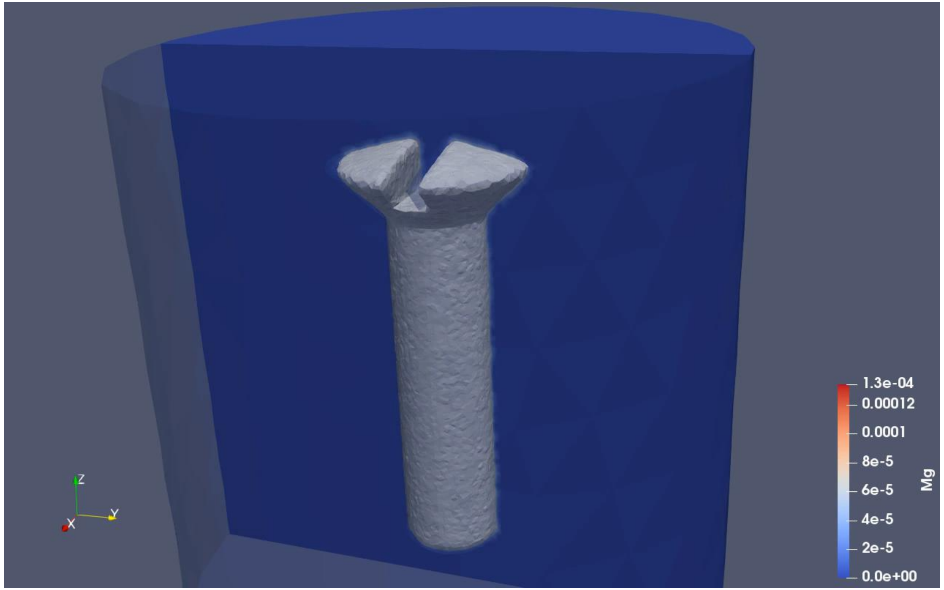
- Not feasible to implement models in sophisticated software packages
- Discretizing PDEs, finite element method
- Level-set for capturing the moving corrosion front
- Adaptively refined mesh generation

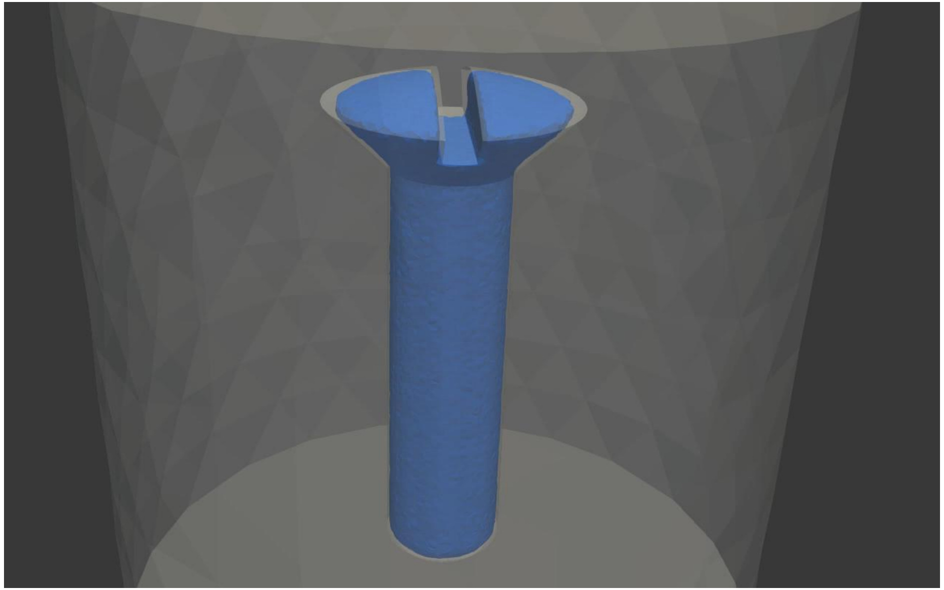


Implementing Computational Model

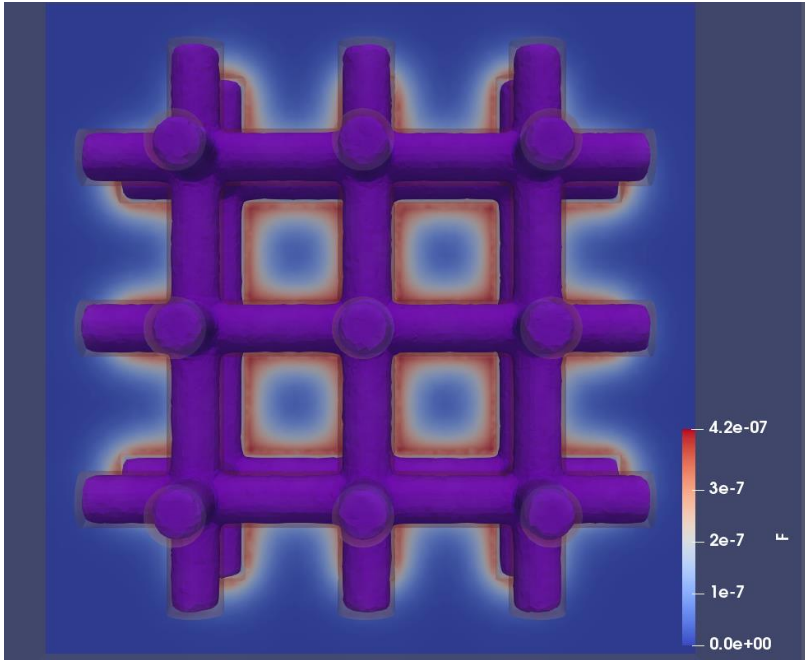
- Mesh generation (SALOME, Mmg), #Element ~ 10M – 20M
- Weak form implementation (FreeFEM), #DoF ~ 2M – 4M
- Parallelization is essential
  - High-performance domain decomposition (HPDDM)
  - High-performance preconditioners and solvers (PETSc)
- Paralleled IO postprocessing (ParaView)

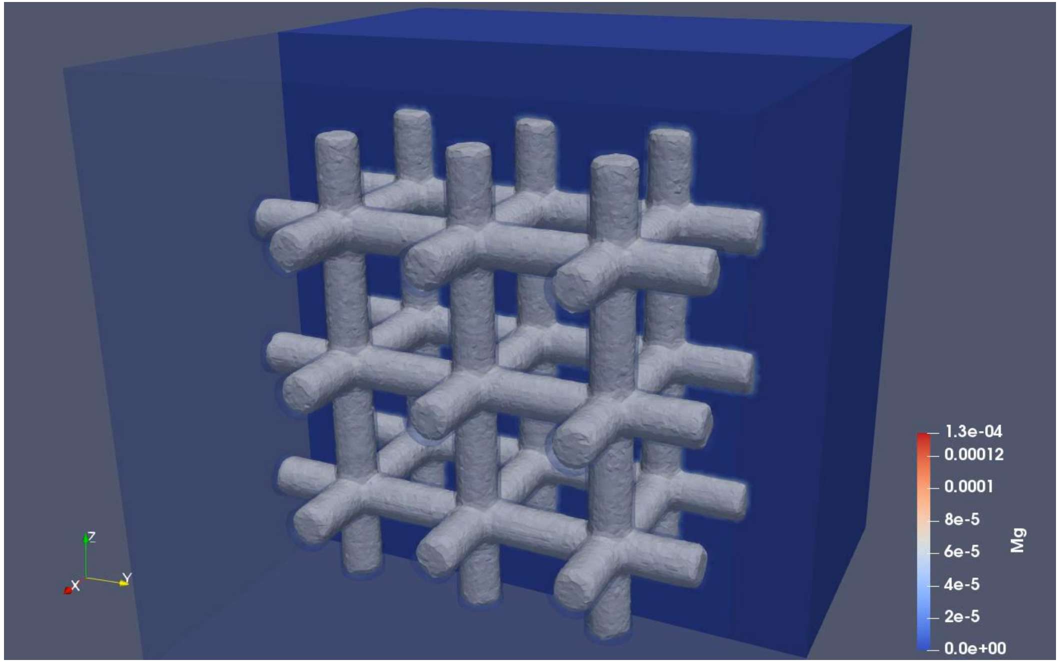
Orthopedics Screw Degradation



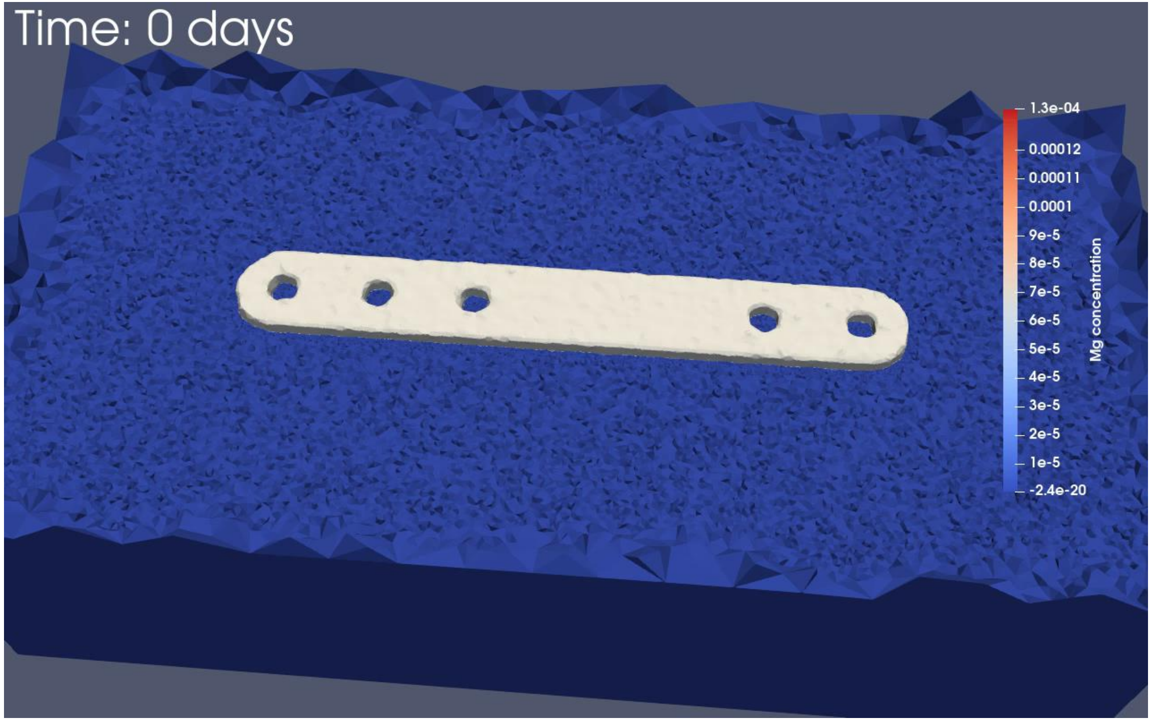


Porous Scaffold Degradation

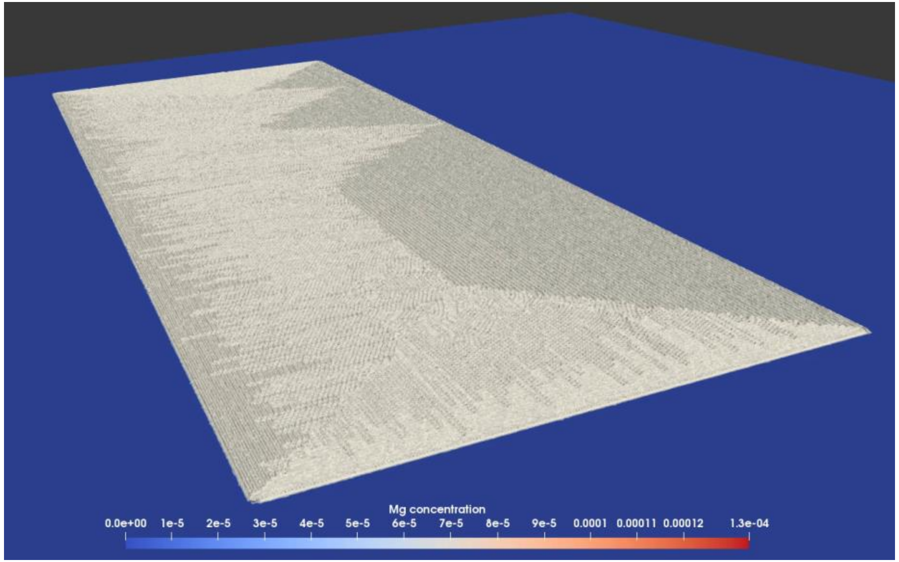


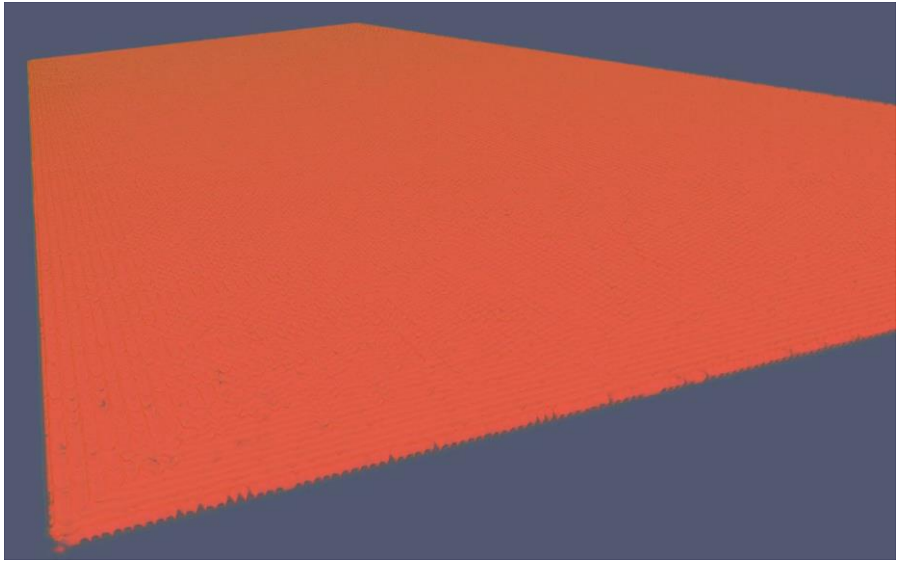


Jaw Bone Plate Degradation



Narrow Cuboid





(Barzegari et al., Corrosion Science, 190, 2021)

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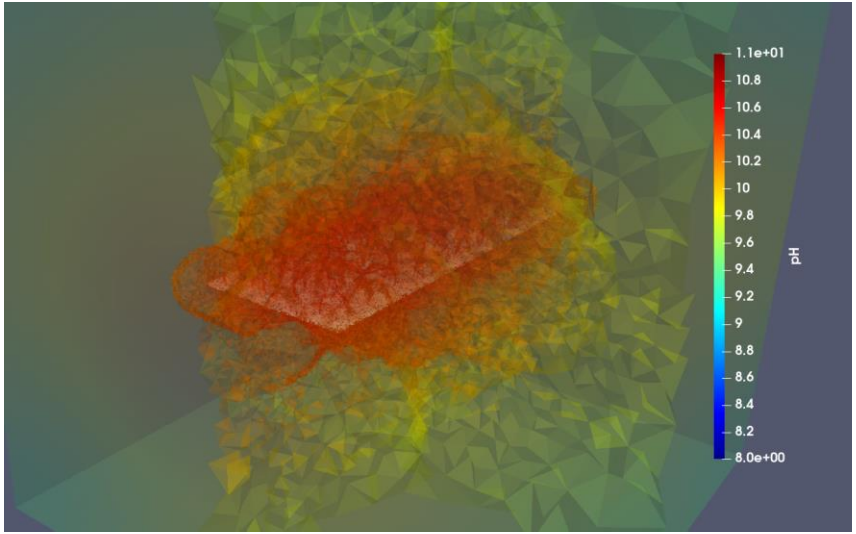
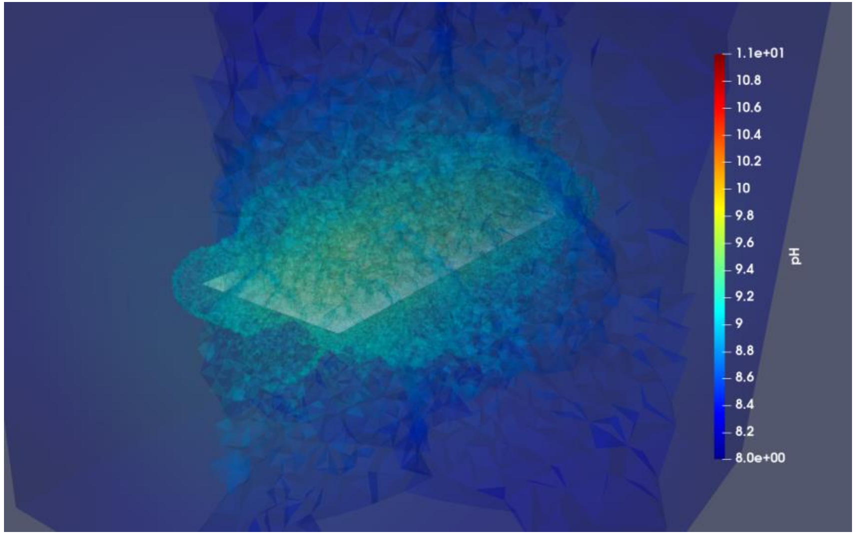
Global pH Change



High diffusion (Saline solution)



Low diffusion (Buffered solution)

(Barzegari et al., Corrosion Science, 190, 2021)

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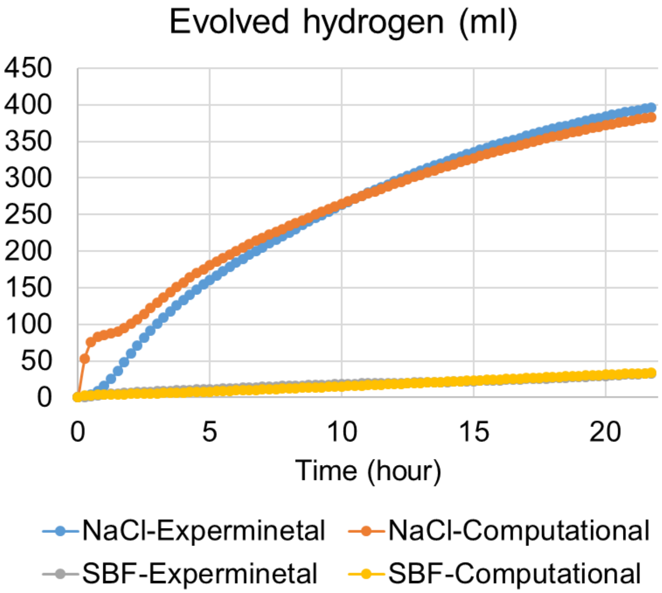
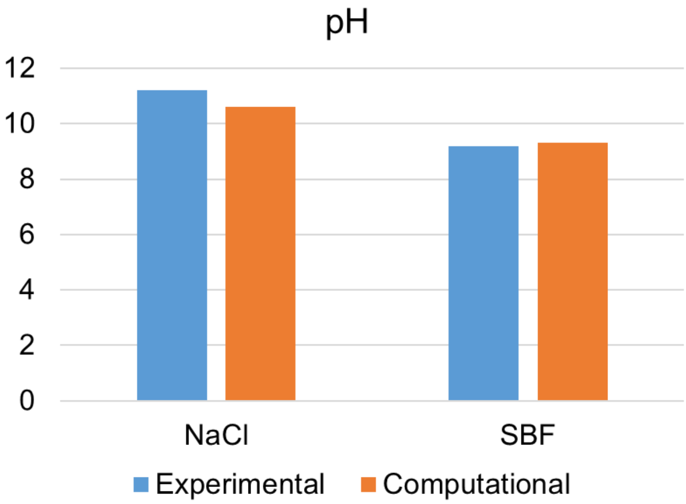
Quantitative Results for Validation





(Barzegari et al., Corrosion Science, 190, 2021)

Adding Perfusion Models (Fluid Flow)

Considering Convection

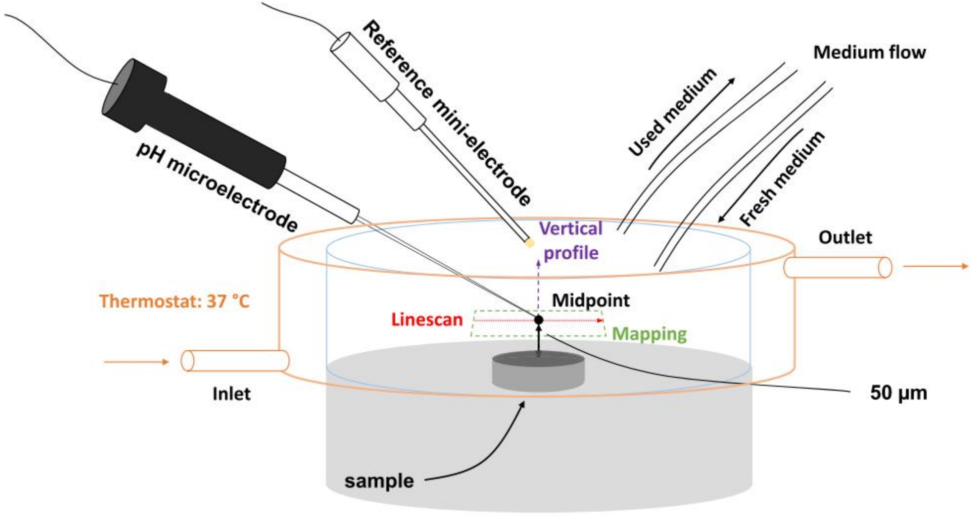
- Adding fluid flow and considering the effect of hydrodynamics condition
- Requires dealing with Navier-Stokes equations

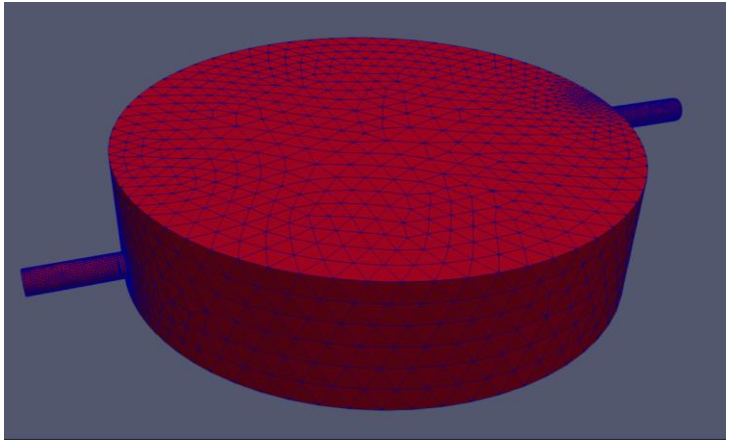
$$\begin{cases} \rho \dfrac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla \mathbf{u}) - \mu \nabla^2 \mathbf{u} + \nabla p = 0 \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

- Implementing a parallel fluid flow code in FreeFEM
- Comparing the output of the CFD code with OpenFOAM (simpleFOAM)

Perfusion Case Simulation Setup

- Degradation in hydrodynamics condition, measuring the local pH

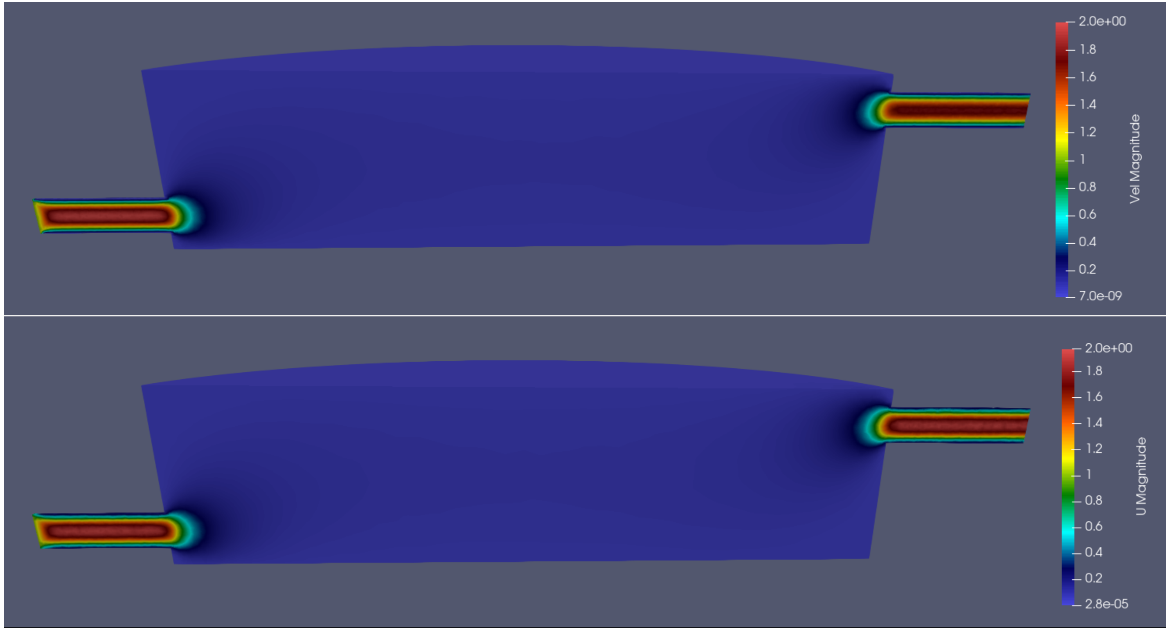




(Wang et al., Corrosion Science, 197, 2022)

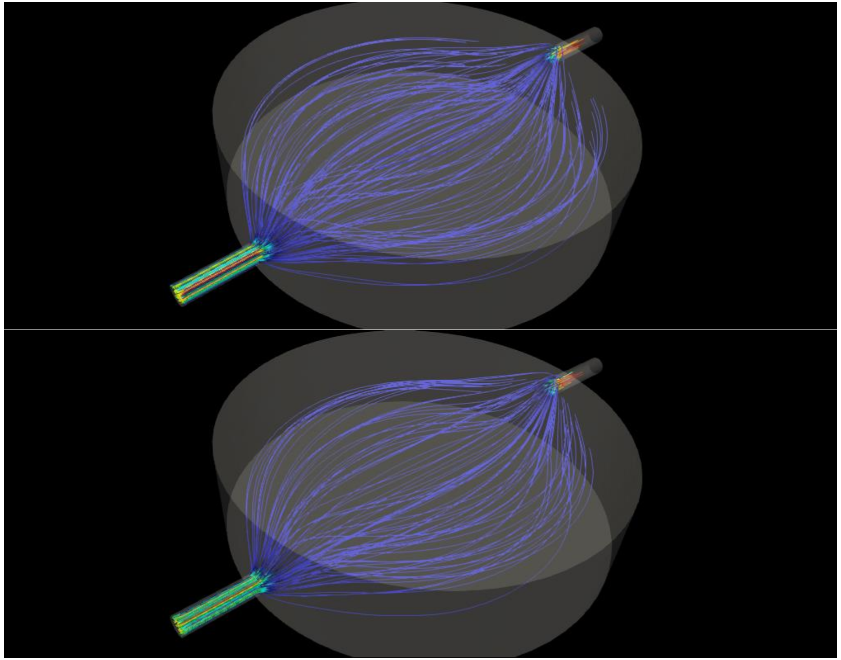
Comparing Fluid Results with OpenFOAM

- Fluid velocity magnitude (top: in-house code, bottom: OpenFOAM)



Comparing Fluid Results with OpenFOAM

- Streamlines, top view (top: In-house code, bottom: OpenFOAM)



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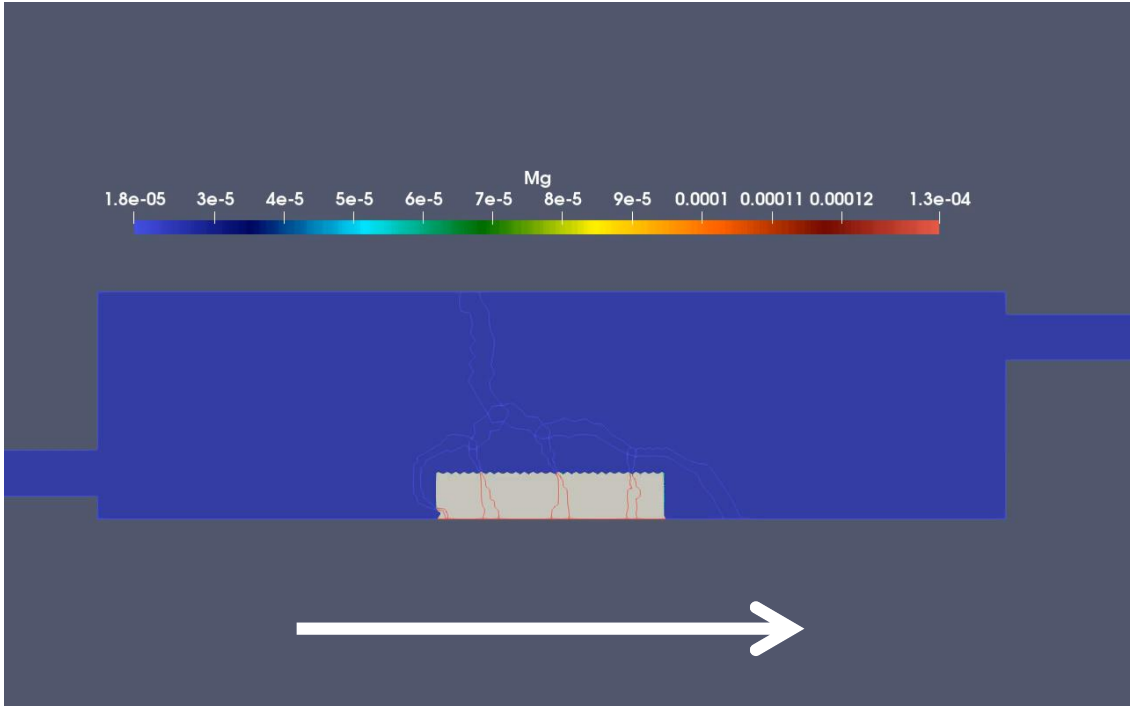
Simulation Results – Degradation with Flow



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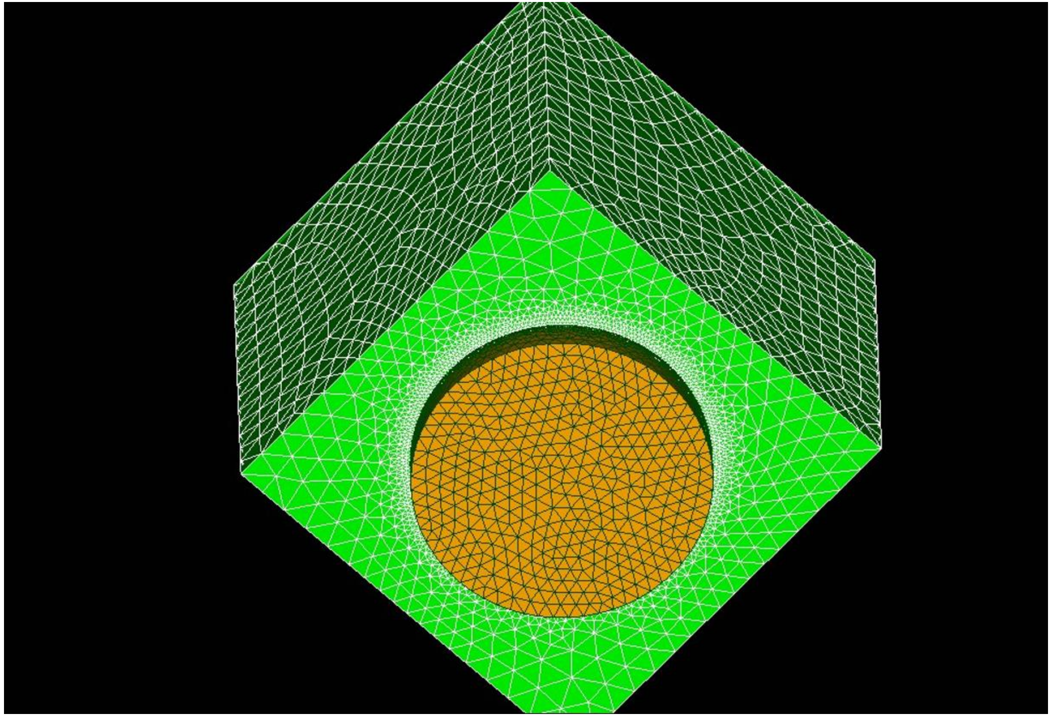
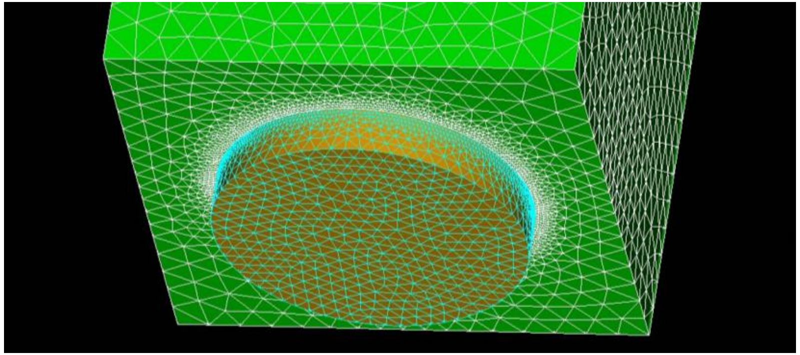
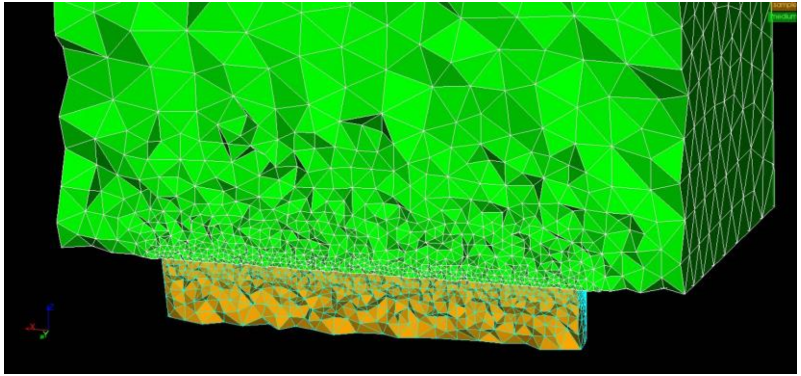
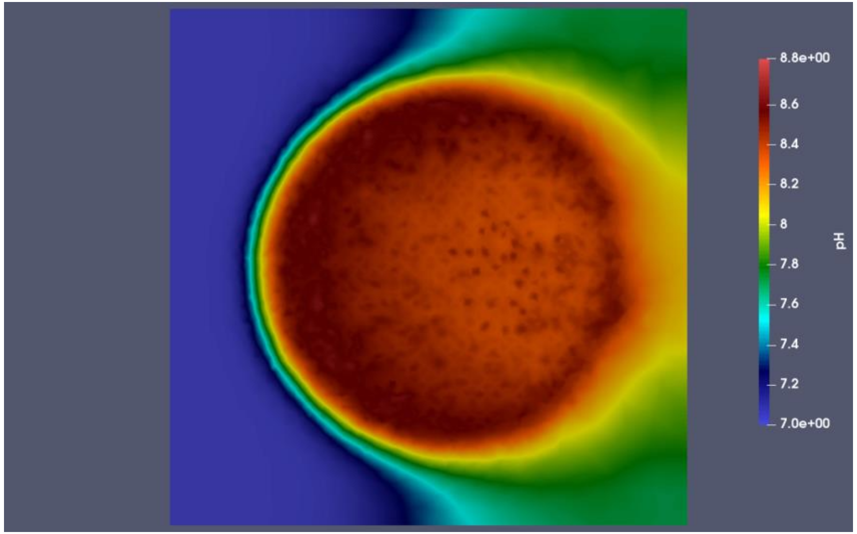
Detailed Model for Local Measurements



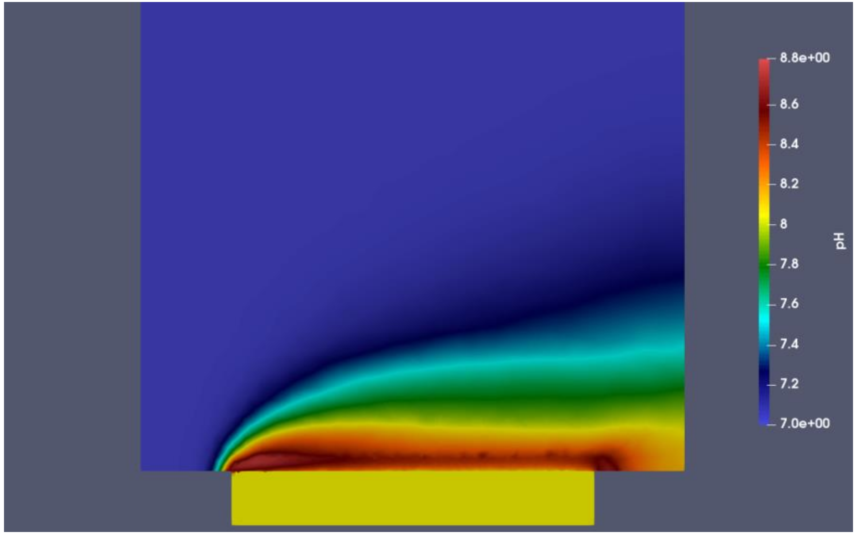




Local pH Change (T=25˚C)

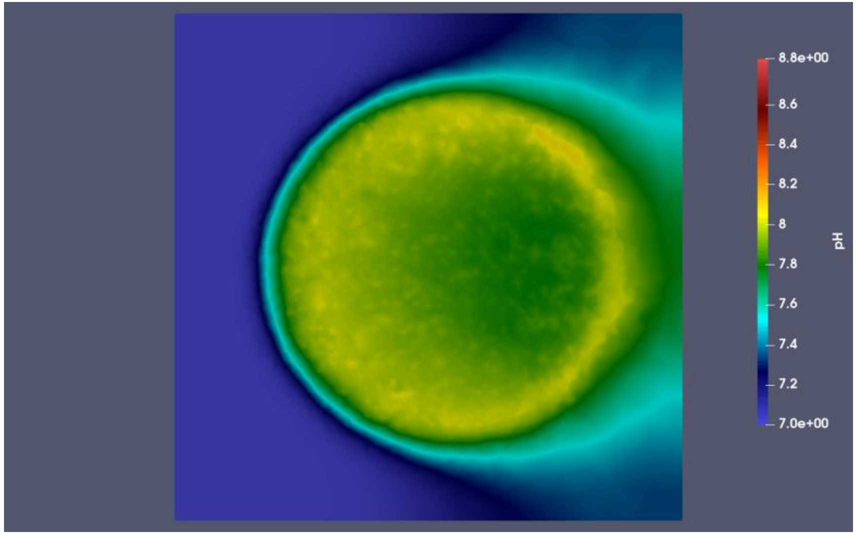


Result from top view

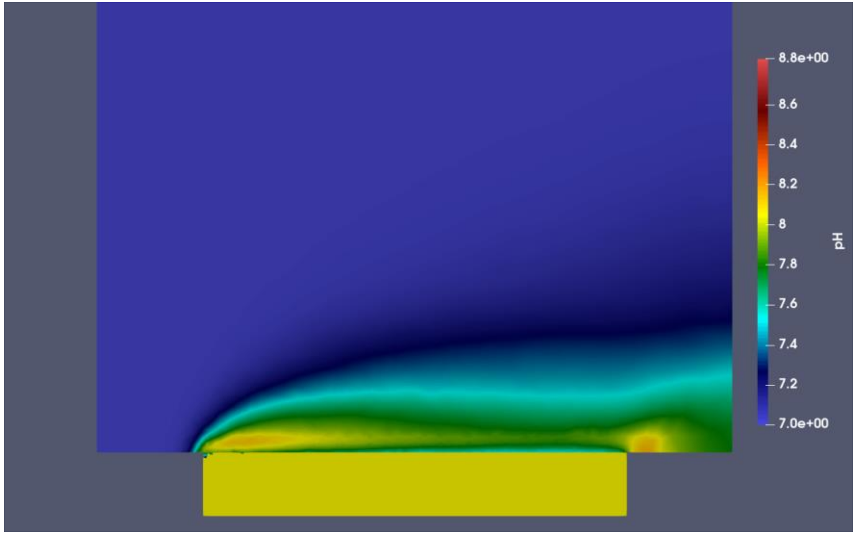


Result from side view

Local pH Change (T=37˚C)



Result from top view



Result from side view

Local pH Changes over Time

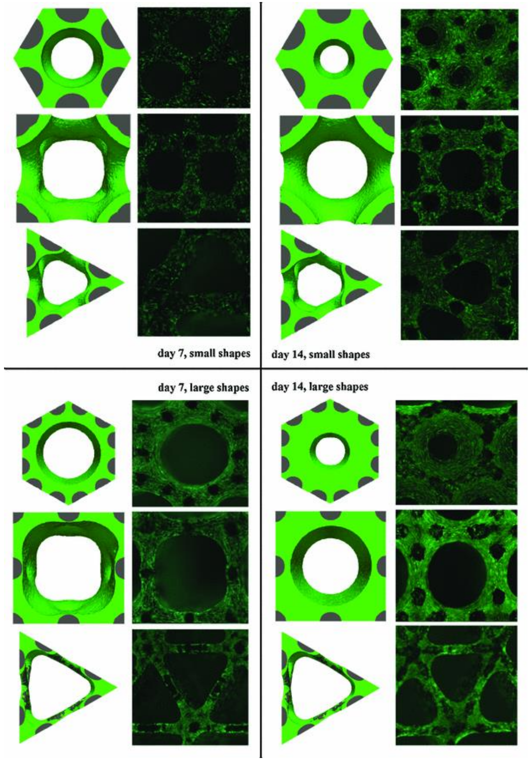
Blue: 25˚C

Red: 37˚C

Tissue Growth Models

Curvature-based Tissue Growth

- Cell growth on open porous scaffolds
- Effect of geometrical characteristics (pore size, shape, and curvature)
- Computational models for the growth of neotissue and cell proliferation process
- Modeling growth as a moving interface problem

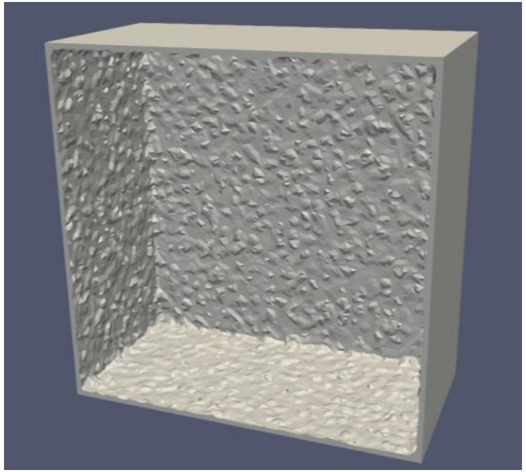


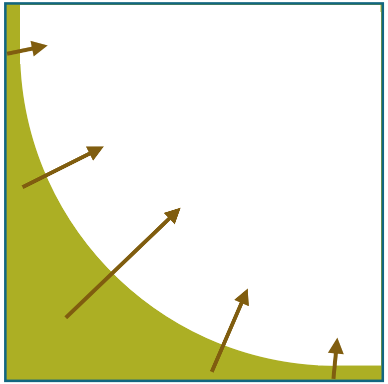
(Guyot et al., Biomech Model Mechanobiol., 13, 2014)

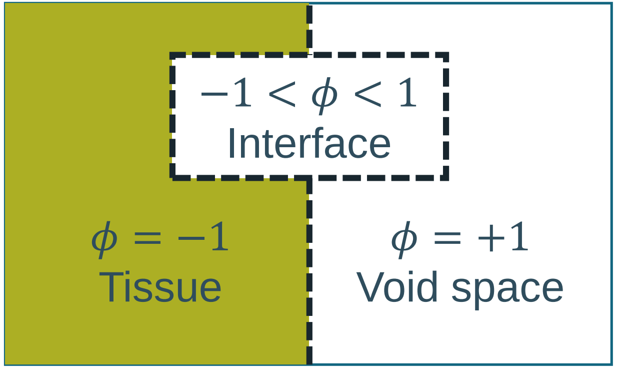
Capturing the Tissue Growth Interface

- Phase field equation for growth

$$\frac{\partial \phi}{\partial t} = b\left[\nabla^2\phi + \frac{\phi(1-\phi^2)}{W^2}\right].\mathrm{H}\left(\nabla^2\phi + \frac{\phi(1-\phi^2)}{W^2}\right)$$



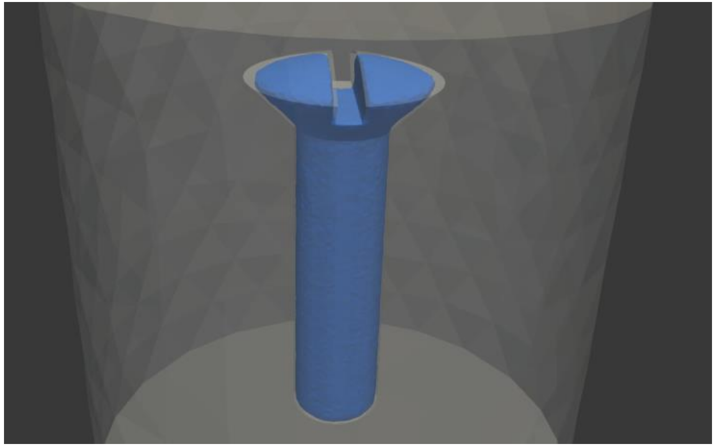


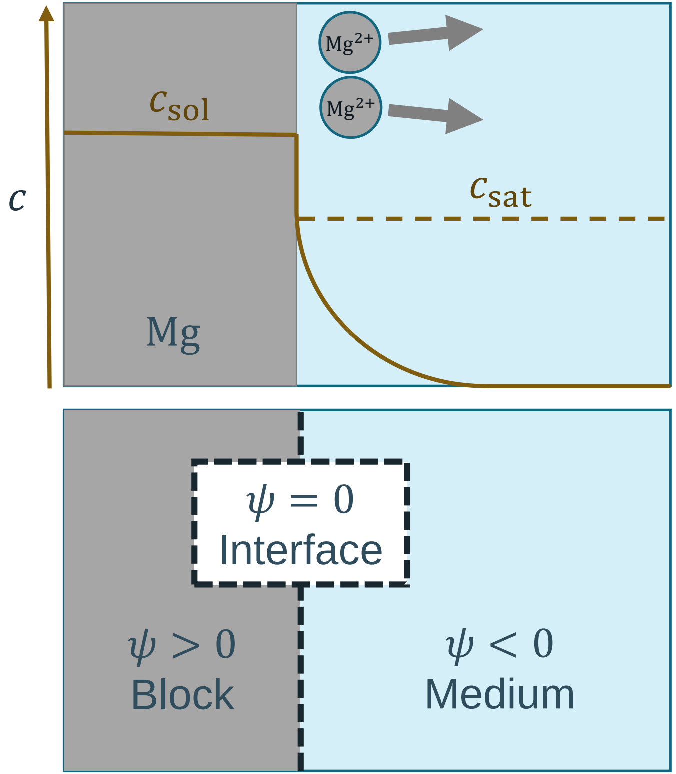


Capturing the Biodegradation Interface

- Level set equation

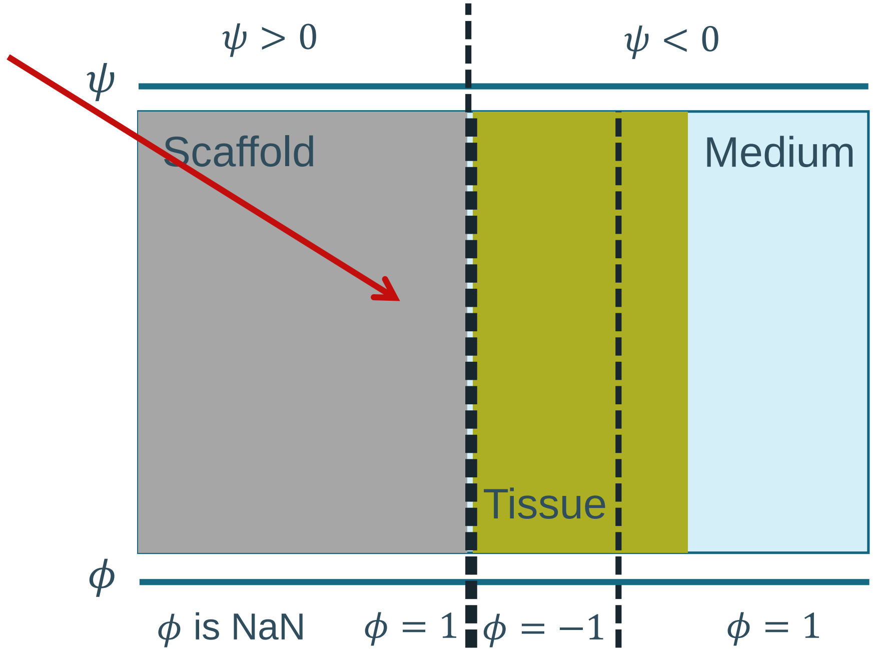
$$\frac{\partial \psi}{\partial t} - \frac{D^{e}_{\mathrm{Mg}} \nabla_n C_{\mathrm{Mg}}}{[\mathrm{Mg}]_{\mathrm{sol}} - [\mathrm{Mg}]_{\mathrm{sat}}} |\nabla \psi| = 0$$





Combining Both Interfaces Together

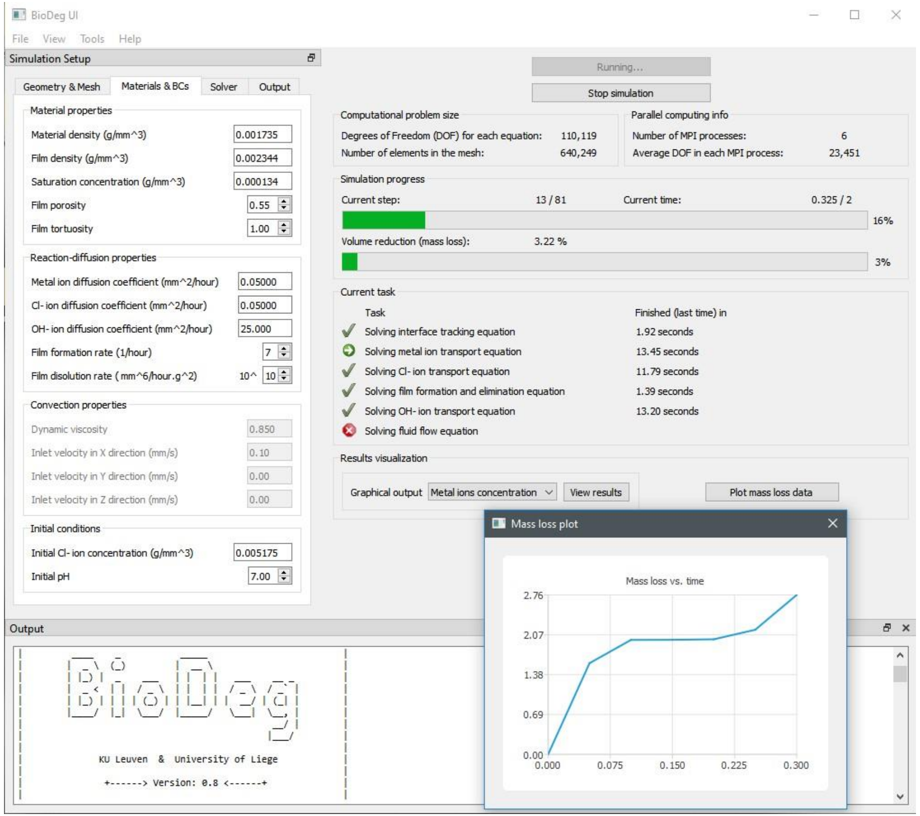
- Having tissue growth on a degrading scaffold
- Issue with this new void space



Software Development & Open-Source

BioDeg Software

- Multifunctional 3D simulation code for modeling biodegradation
- Cross-platform user interface
- Included pre- and post-processors
- FeeFEM/PETSc backend
  Qt/C++ frontend
- Available as an open-source software



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Employed Tools are Open-Source

Mesh Generation

- TetGen
- GMSH
- SALOME
- Mmg

CAD Design

- SALOME
- FreeCAD

PDE Solvers

- FreeFEM
- FEniCS
- OpenFOAM

Sparse Solvers

- MUMPS
- PETSc (GMRES)

Partitioning

- HPDDM
- ParMETIS

Postprocessing

- ParaView
- Medit
- Seaborn

Parallelization

- OpenMPI
- MPICH

Optimization

- HyperOpt
- Spark

Preconditioning

- HYPRE
- PETSc

User Interface

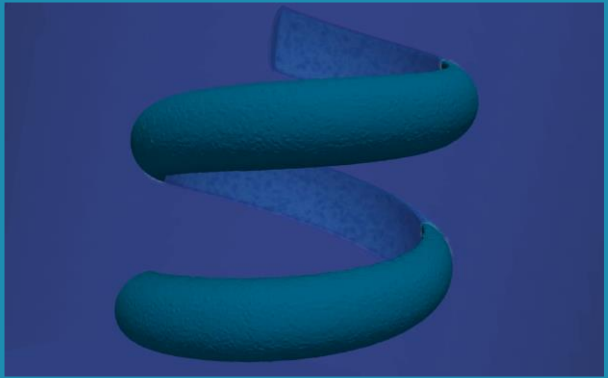
- Qt

Thermodynamics

- Spana

Hosted on GitHub

- BioDeg core (FreeFEM, PETSc) — https://github.com/mbarzegary/BioDeg
- BioDeg UI (Qt, C++) — https://github.com/mbarzegary/BioDeg-UI
- BioDeg pre-processor (FreeFEM) — https://github.com/mbarzegary/BioDeg-preprocess
- BioDeg docs — https://github.com/mbarzegary/BioDeg-doc
- Coupled fluid flow code — https://github.com/mbarzegary/navier-stokes-solver



Thank you for your attention

https://mbarzegary.github.io

@MojBarz

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