# Mathematical modeling of degradation process of biodegradable metallic biomaterials in immersion and perfusion setups

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# 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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# Patient-specific 3D Printed Acetabular Implants

- Implants should be removed at the end of their lifetime
- Some extra bone is also removed along with the implant
- Making at least part of the implant from biodegradable materials

(Source: 3D Systems Inc.)



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# Problem Definition

- Challenge:
  - Tuning the biodegradation to the regeneration of the new tissue/bone
- 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**

**Underlying Science**
- Chemistry of biodegradation
- Physics of perfusion
- Biology of tissue growth

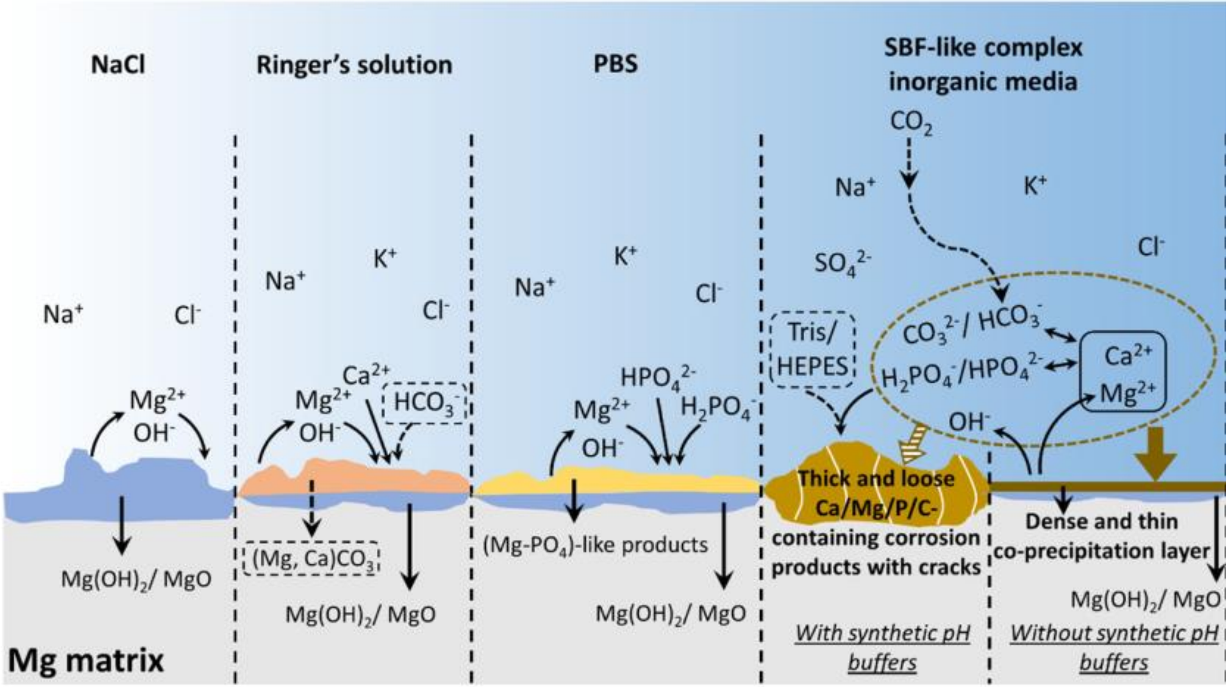
**Mathematical Models**
- Partial differential equations
- Reaction-Diffusion-Convection
- Navier-Stokes equations
- Level set method

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

# Chemistry of Biodegradation

The model captures:

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




(Mei et al., Corrosion Science 171, 2020)



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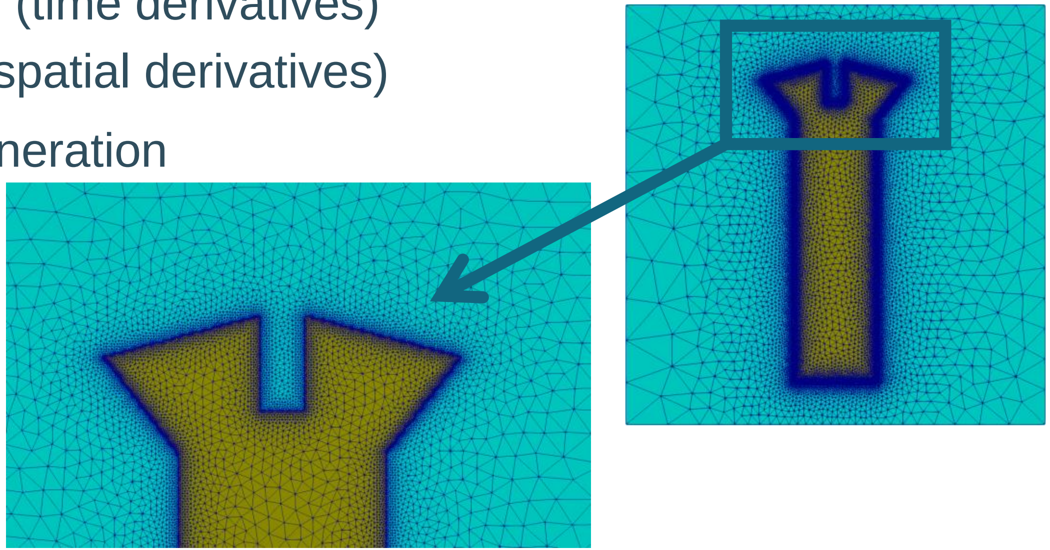
# Constructing Mathematical Model

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

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

# Constructing Computational Model

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





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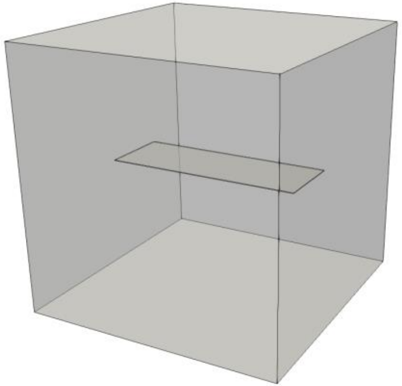
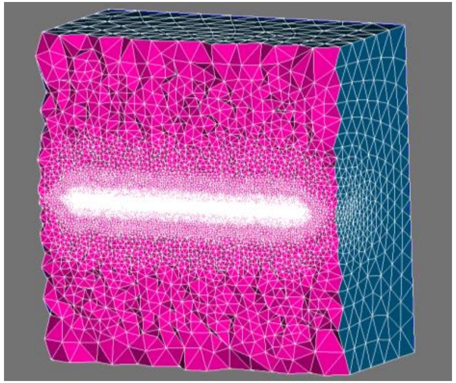
# Immersion Case Simulation Setup

- A narrow cuboid of Mg in SBF/Saline solutions
- Simulating 21 hours of degradation
- Measuring mass loss indirectly via measuring the formed hydrogen
- The global pH is monitored and used to validate the model







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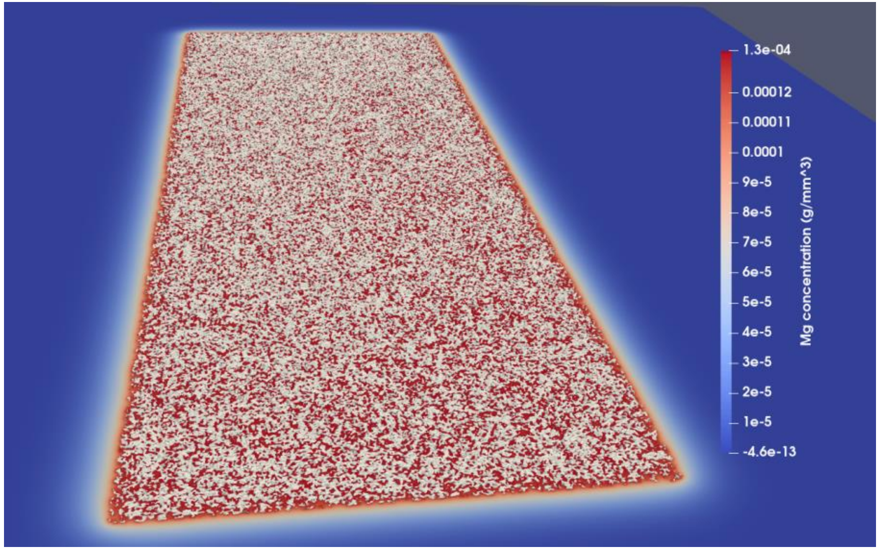
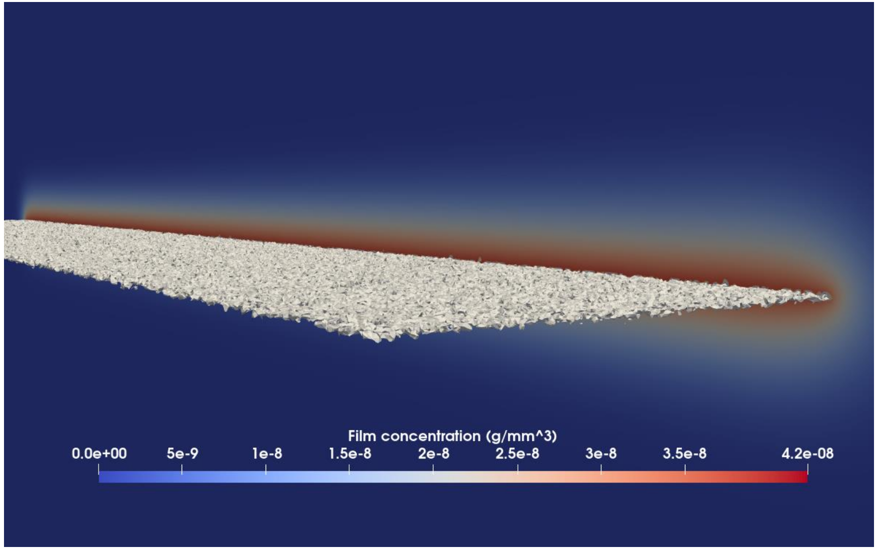
# Simulation Results - Degradation



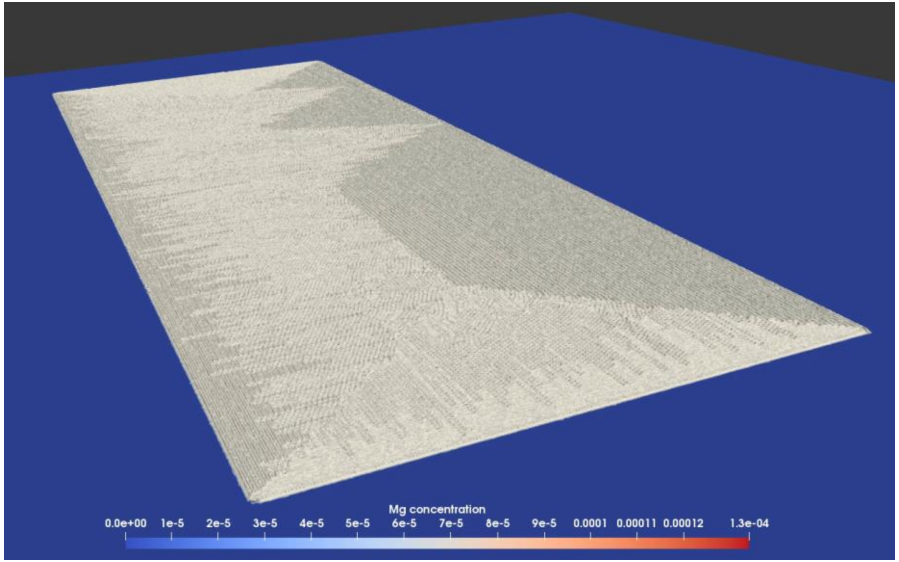

Release of Mg ions

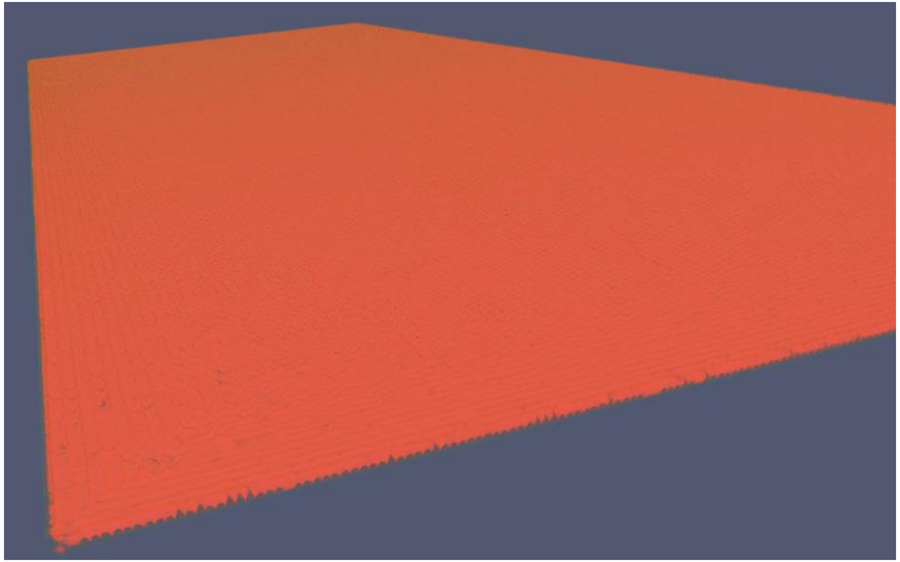



Formation of the protective film

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

# Simulation Results - Degradation



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



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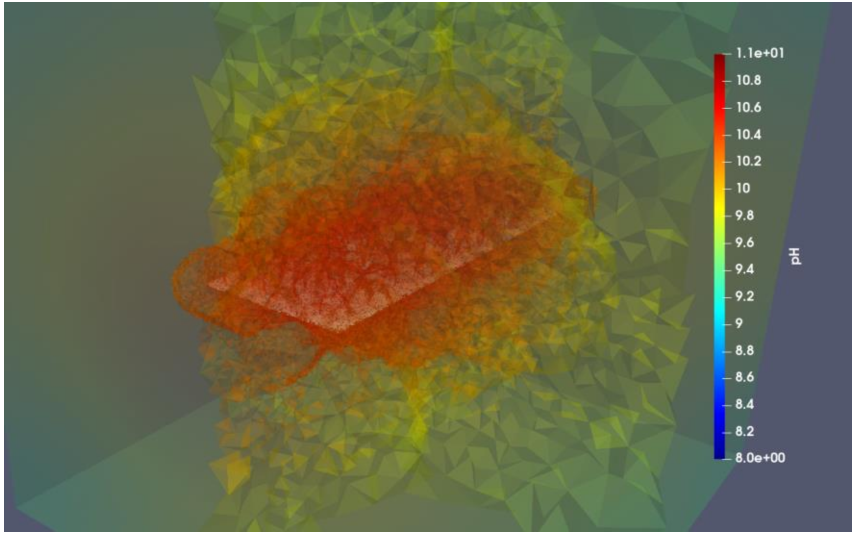
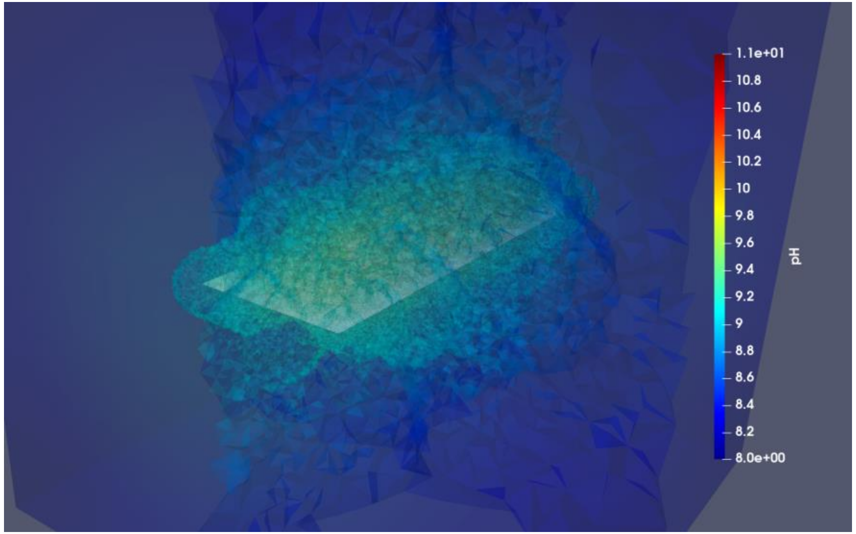
# Simulation Results - pH Change




High diffusion (NaCl solution)




Low diffusion (SBF solution)

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



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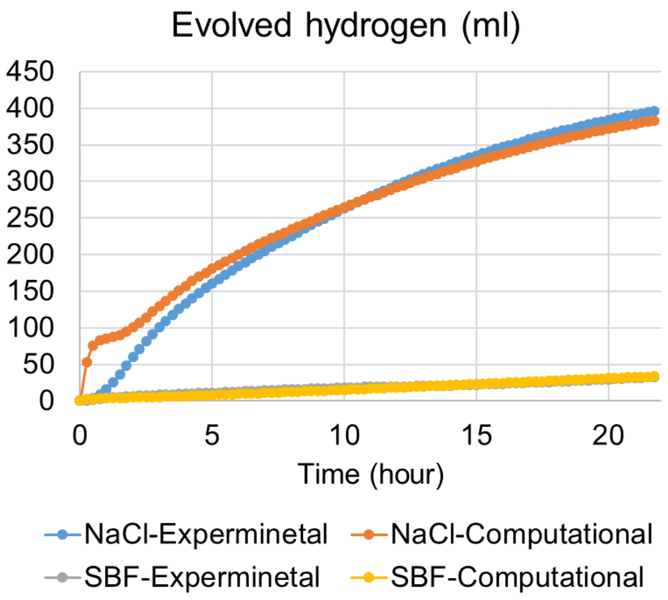
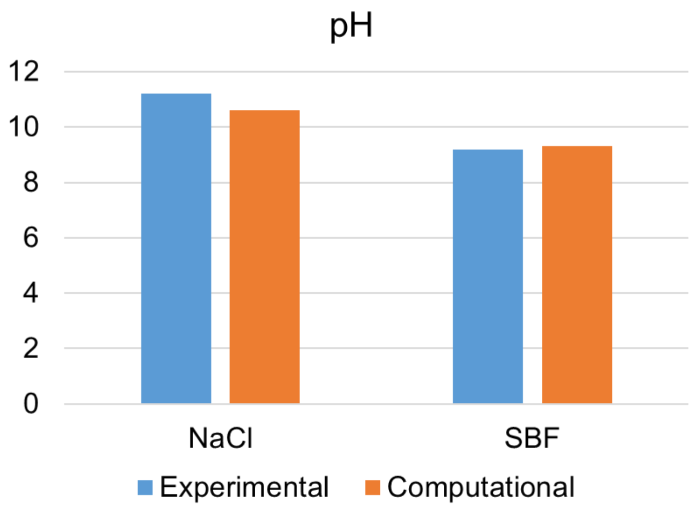
# Quantitative Results




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



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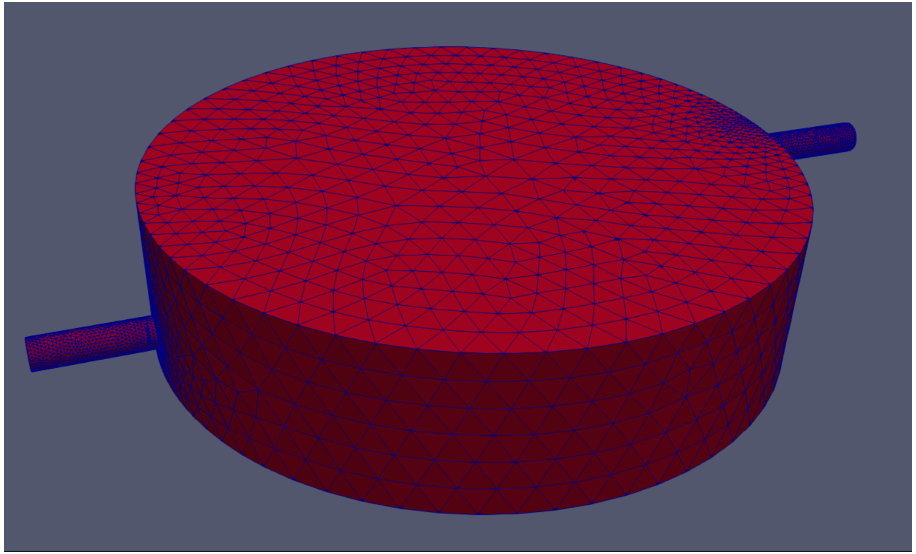
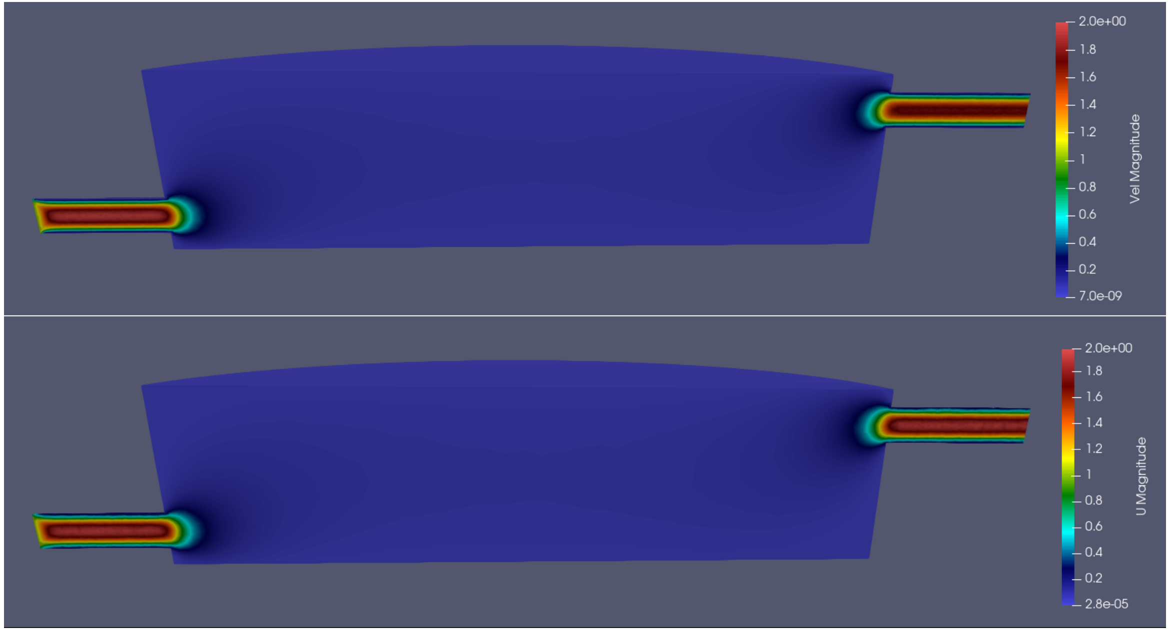
# Perfusion Case Simulation Setup

- Adding fluid flow and considering the effect of hydrodynamics condition
- Degradation inside a chamber with inlet and outlet
- Making sure that the CFD code works correctly



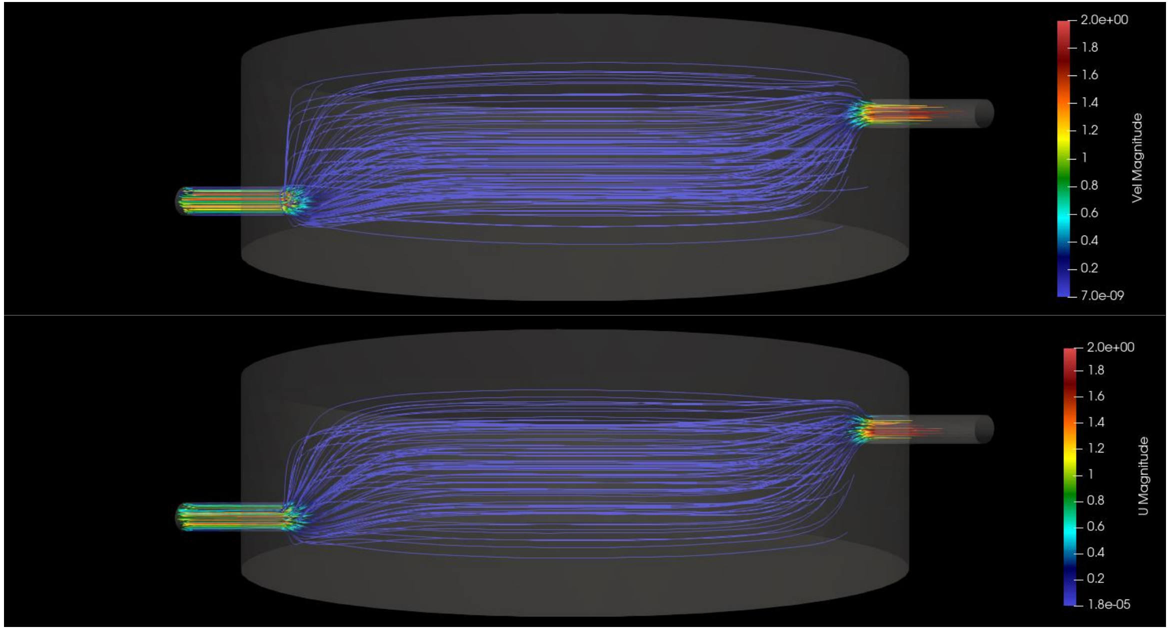
# Comparing Fluid Results with OpenFOAM

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



# Comparing Fluid Results with OpenFOAM

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



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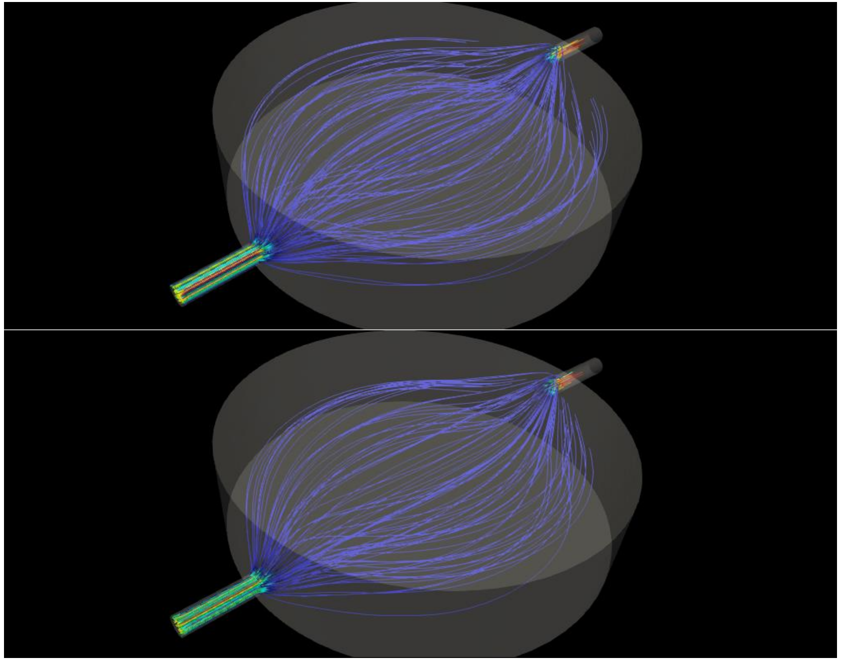
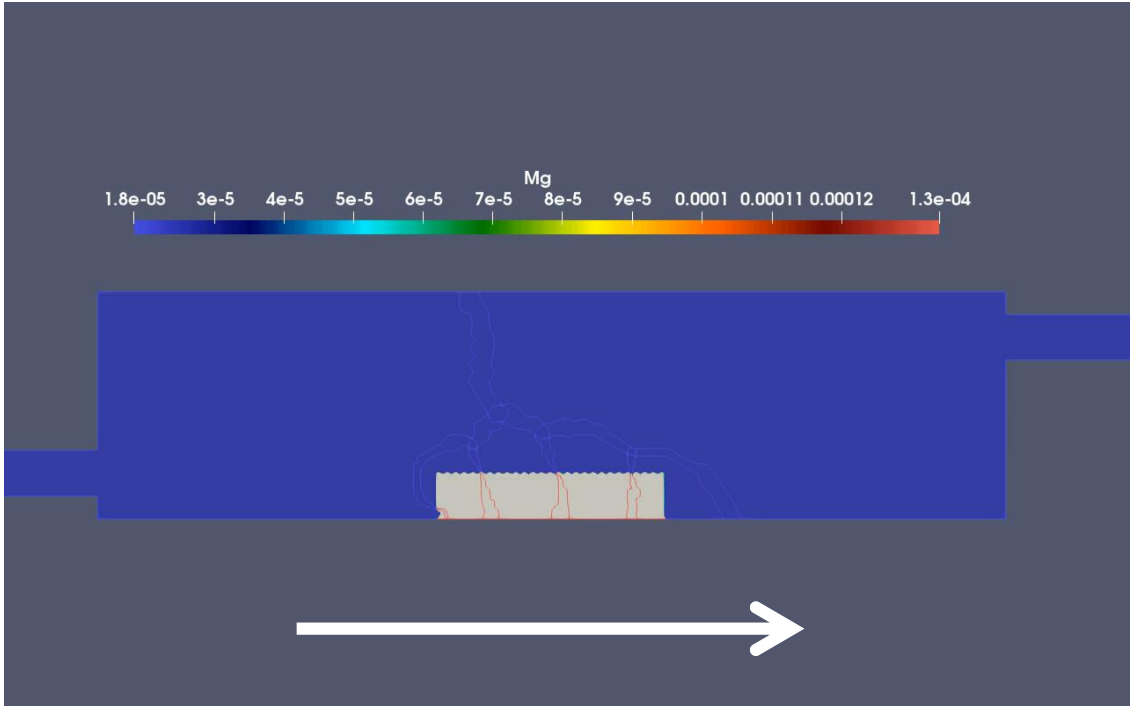
# Comparing Fluid Results with OpenFOAM

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



# Simulation Results – Degradation with Flow



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# Developed Code & Employed Tools are Open-Source

**Mesh Generation**

- TetGen
- GMSH
- SALOME
- MMG

**CAD Design**

- SALOME
- FreeCAD

**PDE Solvers**

- FreeFEM

**Sparse Solvers**

- MUMPS
- PETSc (GMRES)

**Partitioning**

- HPDDM
- ParMETIS

**Postprocessing**

- ParaView
- Medit
- Seaborn

**Parallelization**

- OpenMPI
- MPICH

**Optimization**

- HyperOpt
- Spark

**Preconditioning**

- HYPRE
- PETSc (fieldsplit)

**FE Solvers**

- Code Aster

https://github.com/mbarzegary/BioDeg

# Conclusion

- A quantitative mathematical model to assess the degradation behavior of biodegradable metallic implants in-silico
- Capturing the effect of fluid flow to model hydrodynamics conditions
- By predicting the biodegradation behavior, the model can improve current workflows of designing biodegradable orthopedics implants

# Thank you for your attention!

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