Massively parallel finite element simulation of reaction-diffusion systems with moving boundaries: a use-case for biomaterials degradation modeling

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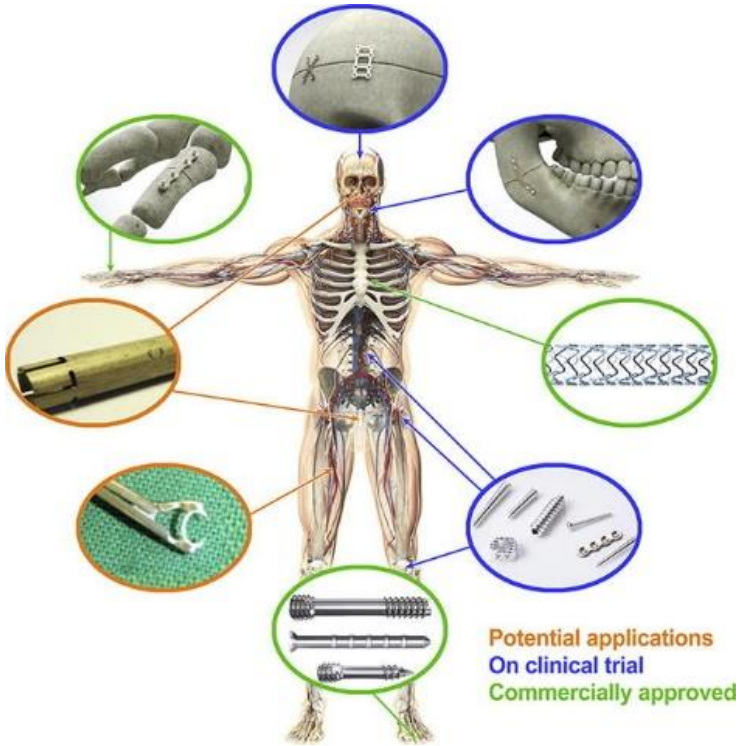
Statement of Need
& Basic Concepts

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

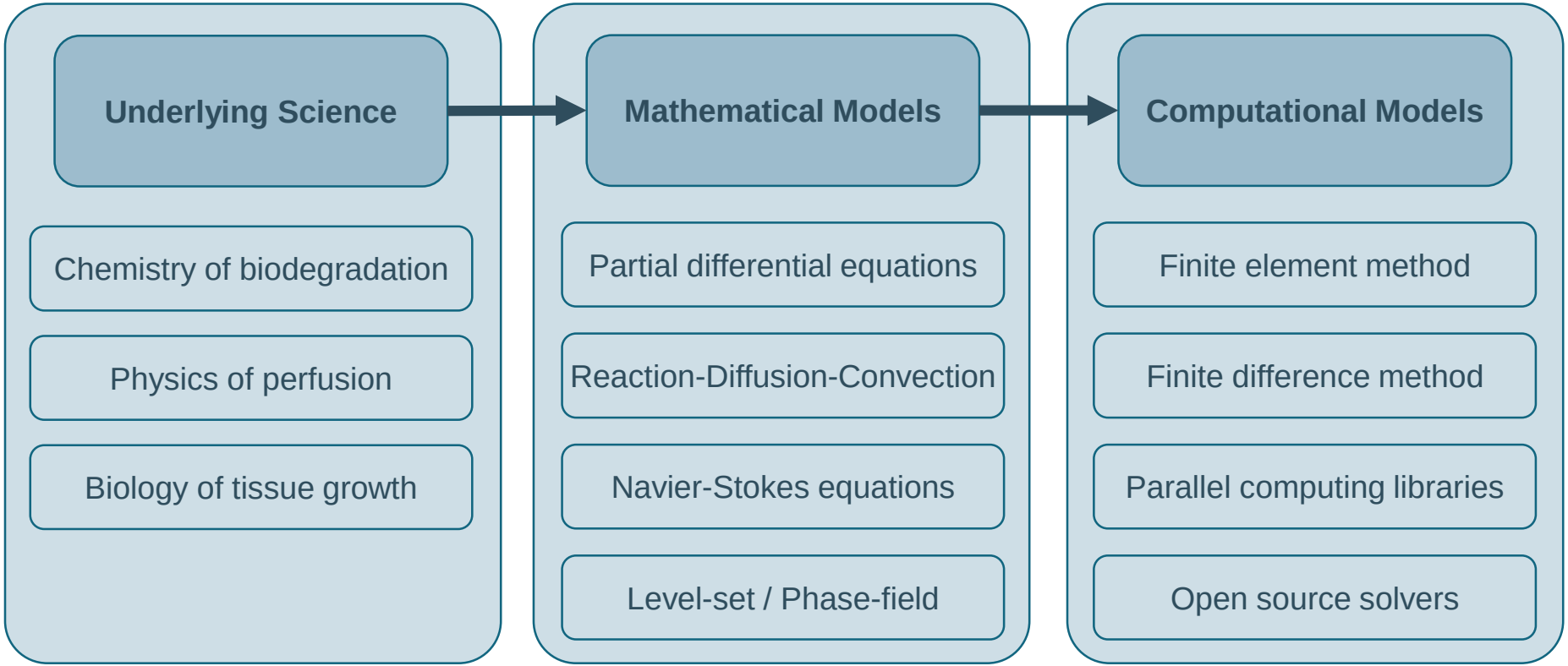


(Han et al., Mater. Today, 23, 2019)

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

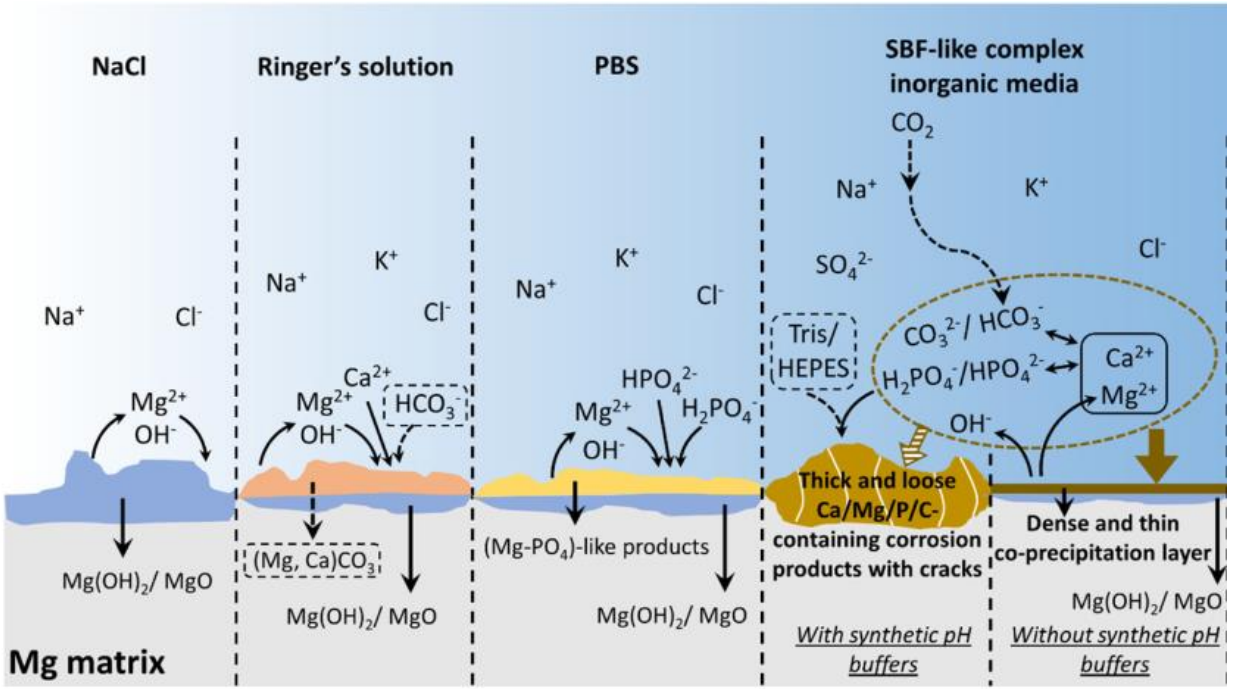
Modeling Workflow



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)

Constructing Mathematical Model

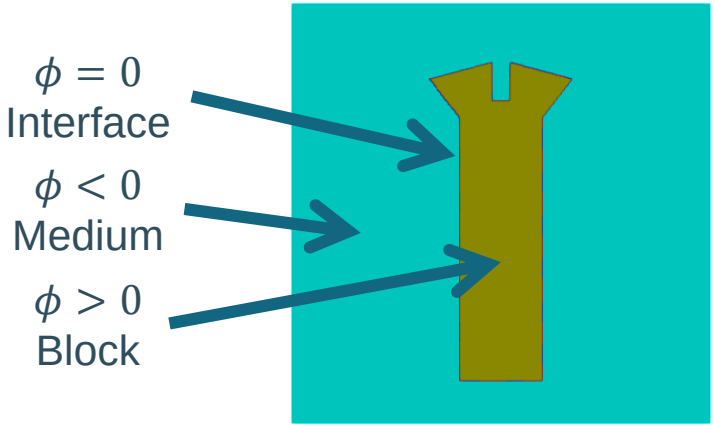
- Converting the chemical interaction into mathematical forms
- Reaction-diffusion-convection partial differential equations (PDE)
- An example for the transport of Mg ions

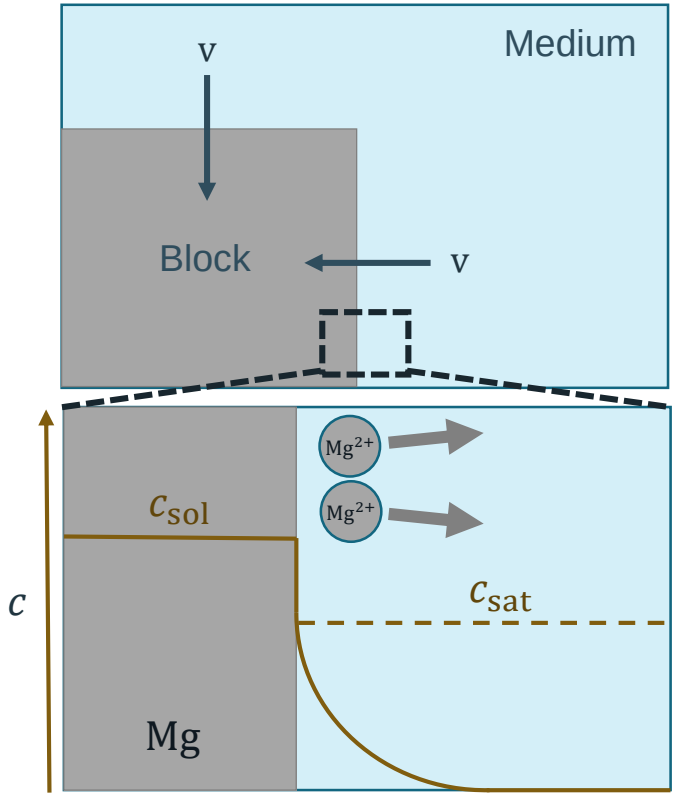
$$\frac{\partial C_{\mathrm{Mg}}}{\partial t} = \underbrace{\nabla.\left(D^{e}_{\mathrm{Mg}} \nabla C_{\mathrm{Mg}}\right)}_{\text{Diffusion}} - \underbrace{\nabla.\left(\mathrm{v} C_{\mathrm{Mg}}\right)}_{\text{Convection}} - \underbrace{k_1 C_{\mathrm{Mg}} \left(1 - \beta \frac{C_{\mathrm{Film}}}{[\mathrm{Film}]_{\mathrm{max}}}\right)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

Capturing the Moving Boundary

- Implicit tracking of the moving corrosion front
- Level set method

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





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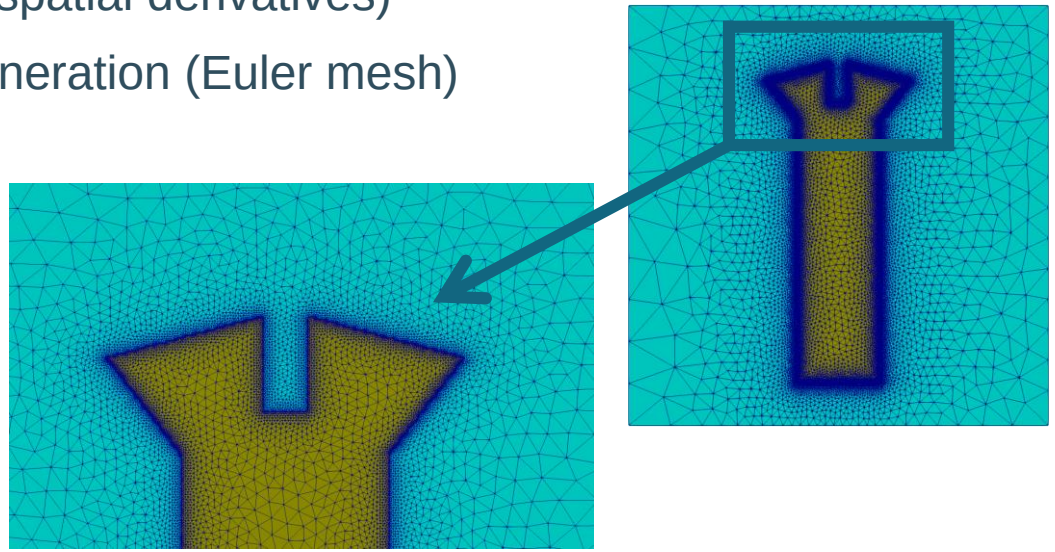
Computational Model Implementation

Constructing Computational Model

- Discretizing PDE equations, numerical computation
  - Finite difference method (temporal derivatives)
  - Finite element method (spatial derivatives)
- Adaptively refined mesh generation (Euler mesh)



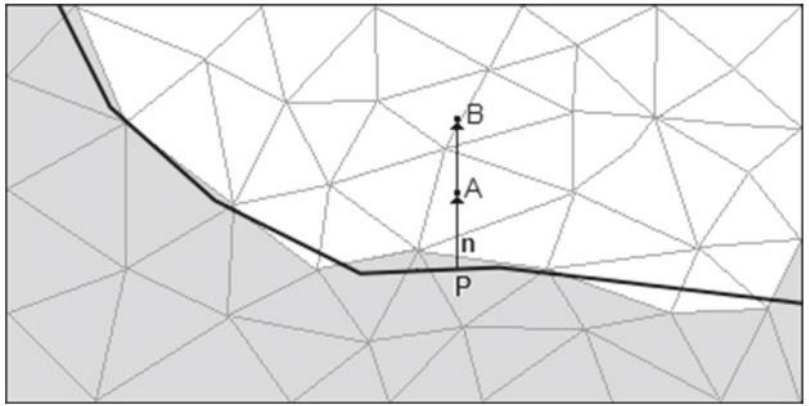
Implementing Computational Model

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

Level Set Implementation

- Penalization for interface BCs
- Problem of concentration oscillation
- Computing $\nabla_n C_{\mathrm{Mg}}$ correctly
- Problem of re-distancing the distance function ϕ

$$\nabla_n C = \frac{C(\mathbf{x} + h.n) - C(\mathbf{x} + 2h.n)}{h},$$
$$\mathbf{x} \in \Omega \subset \mathbb{R}^3$$



(Bajger et al., Biomech. Model., 2017)

Considering Convection

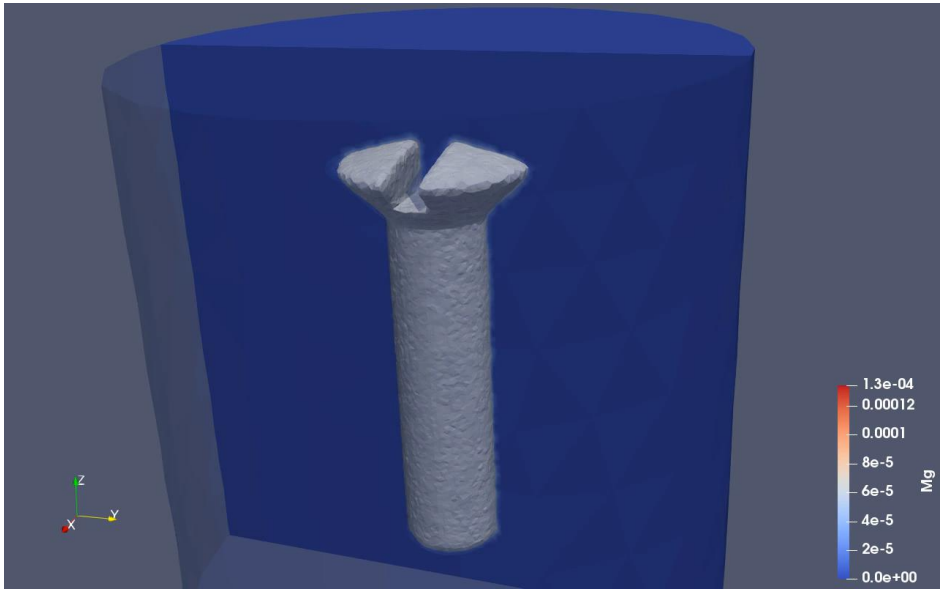
- Adding fluid flow and considering the effect of hydrodynamics condition
- Requires dealing with Navier-Stokes equations

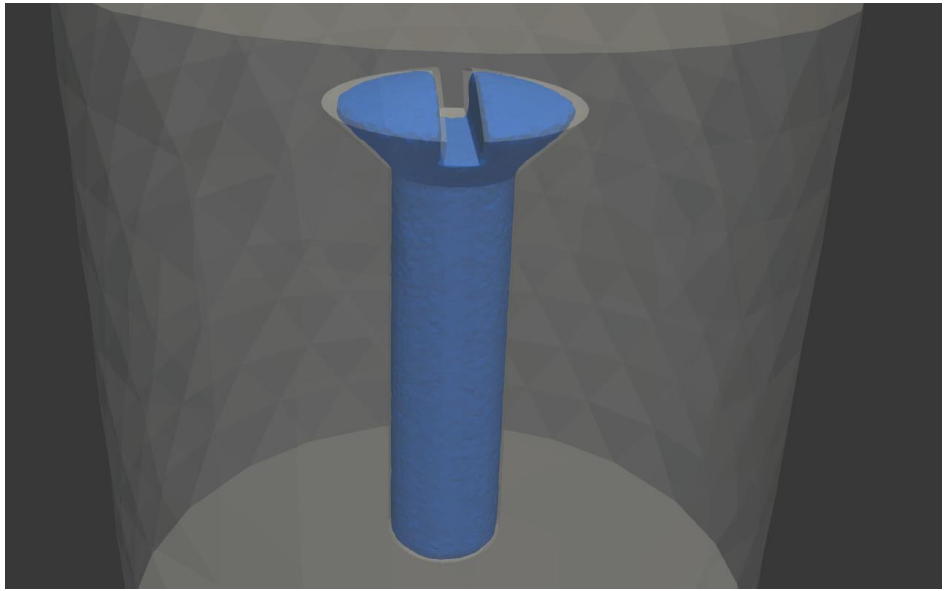
$$\begin{cases} \rho \dfrac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla \mathbf{u}) - \mu \nabla^2 \mathbf{u} + \nabla p = 0 \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

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

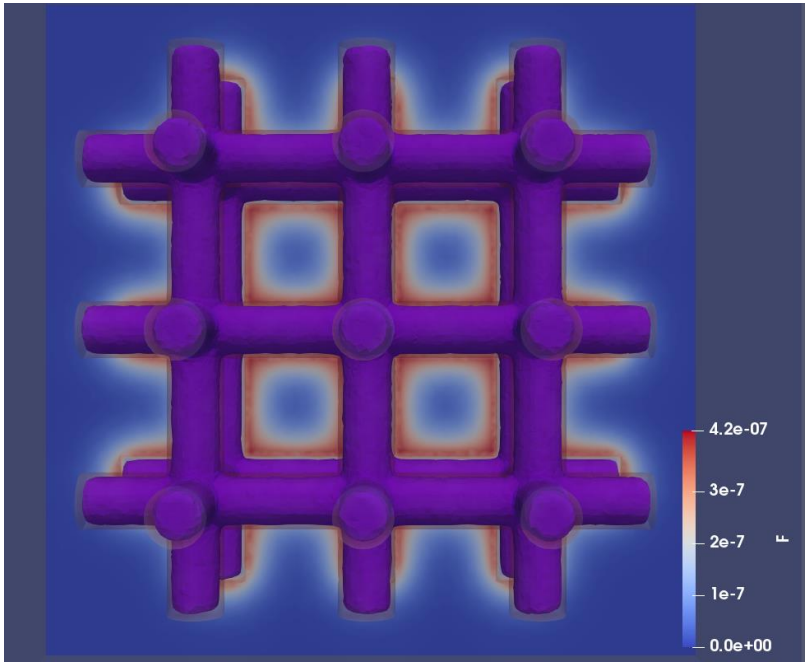
Simulation Results

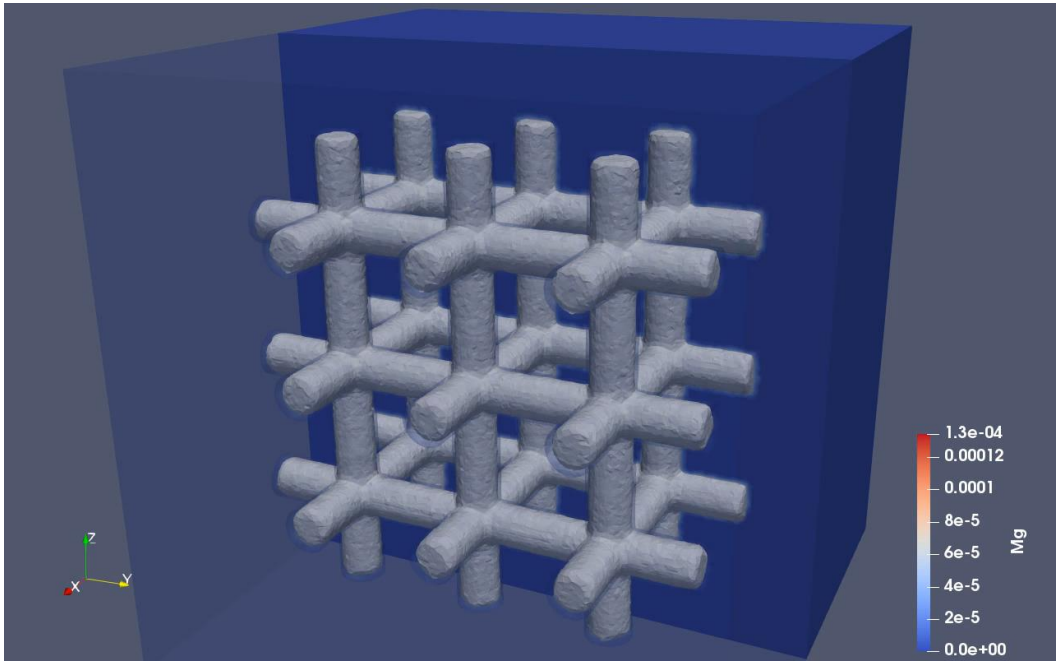
Orthopedics Screw Degradation



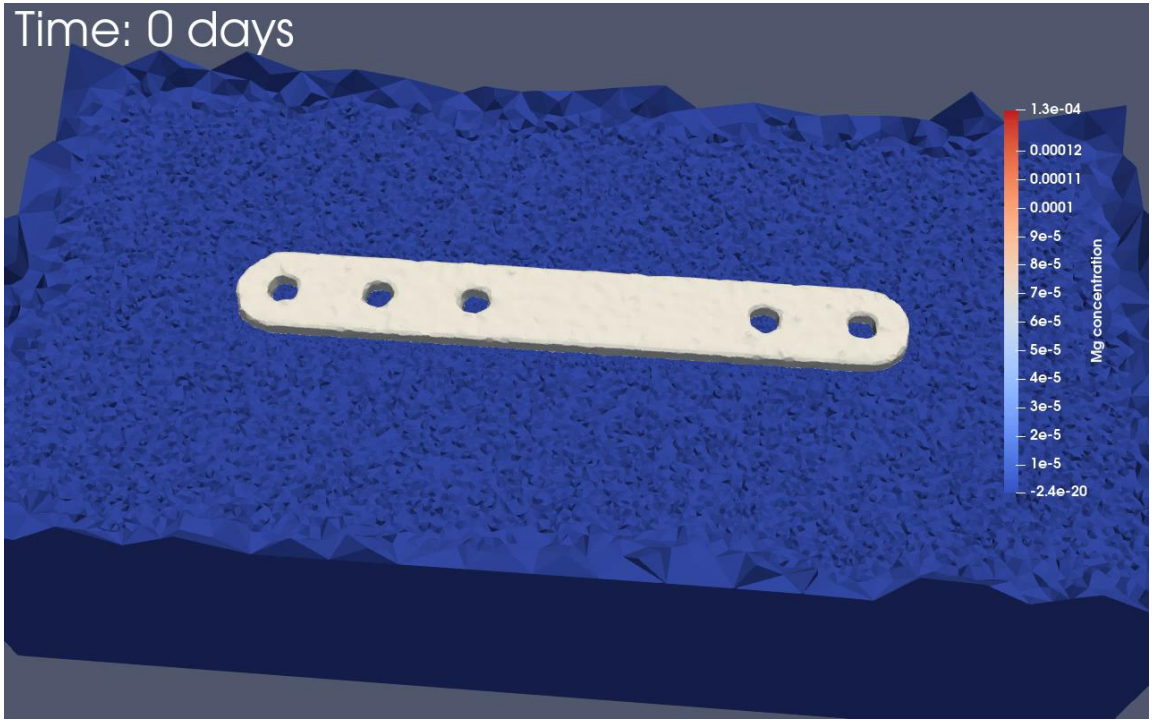


Porous Scaffold Degradation

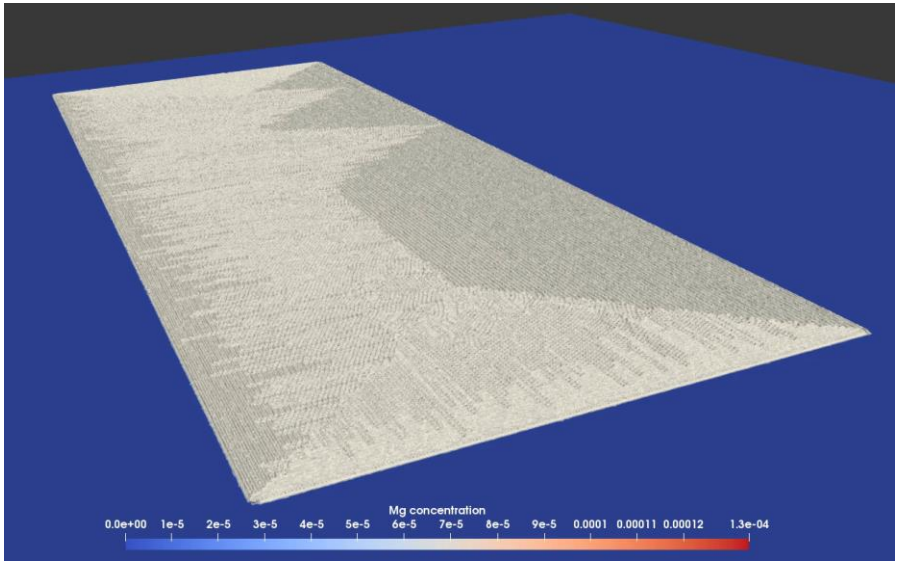


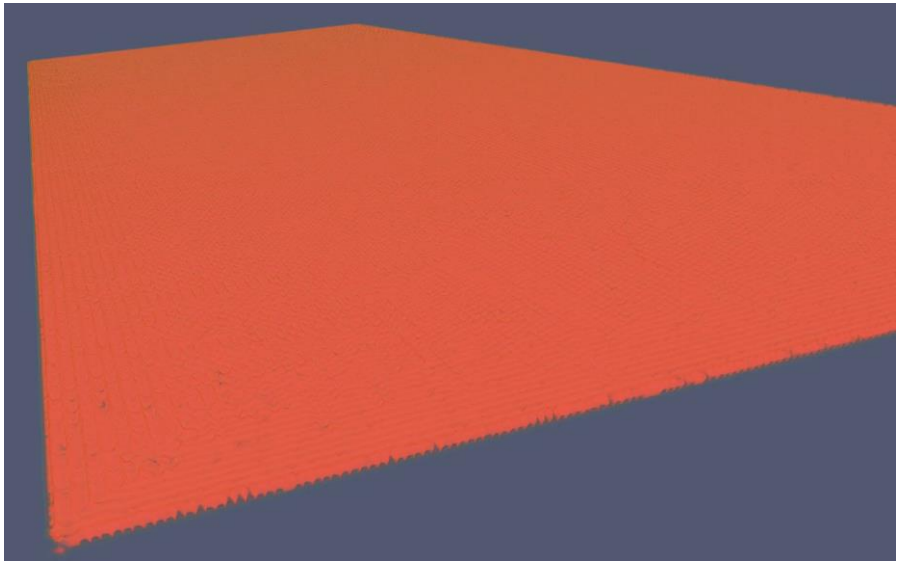


Jaw Bone Plate Degradation



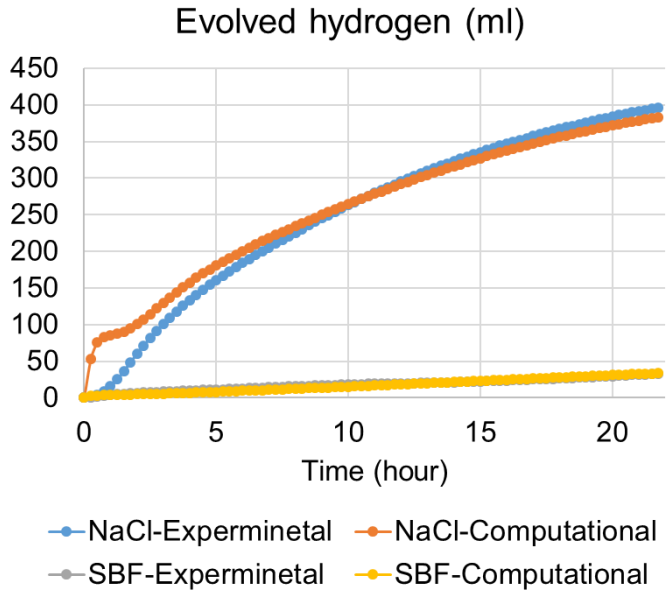
Narrow Cuboid

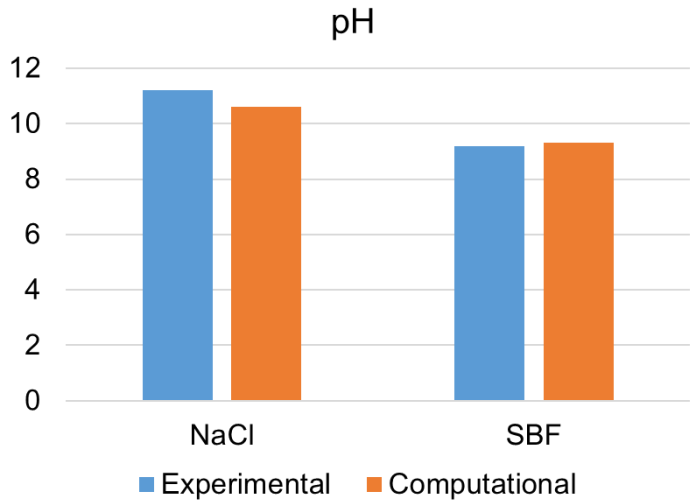




(Barzegari et al., Corrosion Science, 190, 2021)

Quantitative Results for Validation





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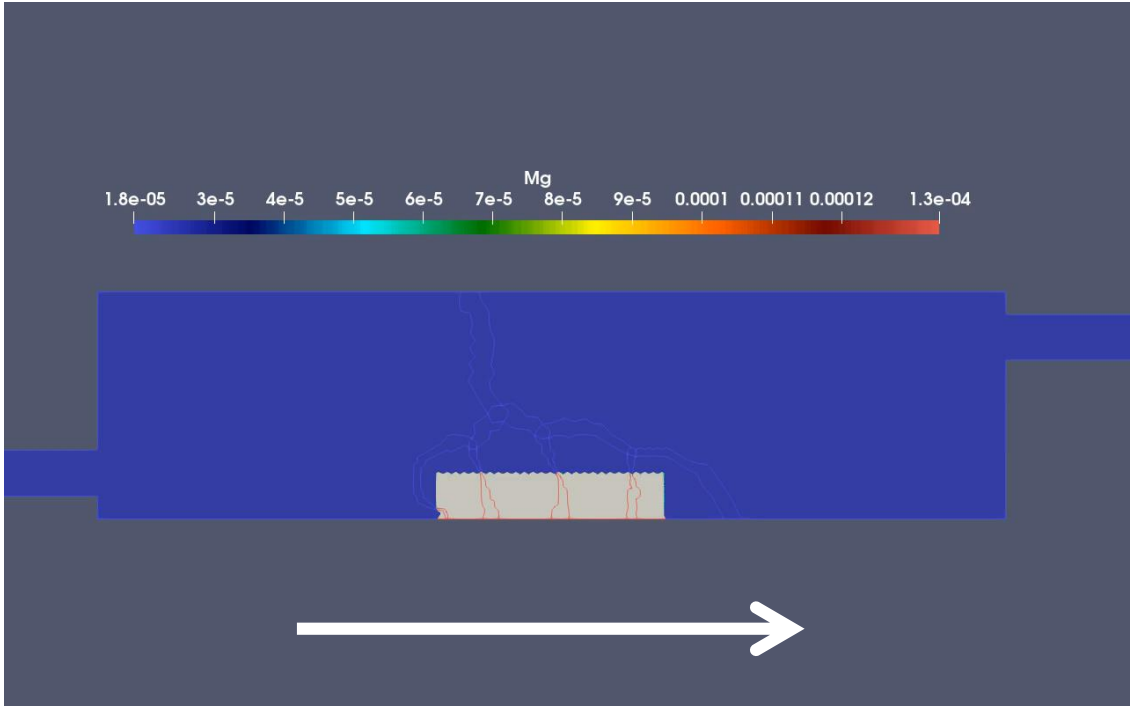
Degradation with Flow



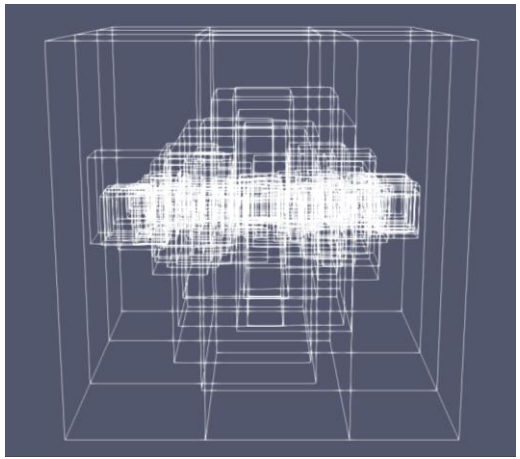
High-Performance Computing

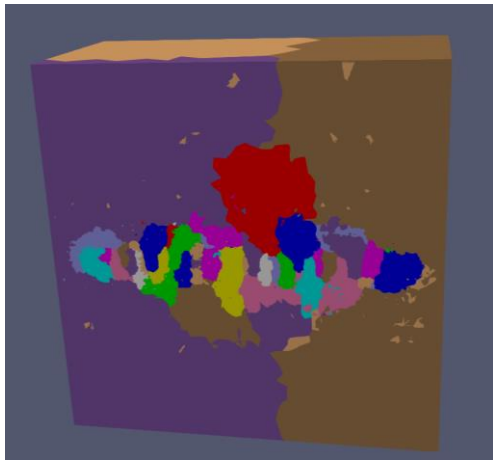
High-Performance Computing Approach

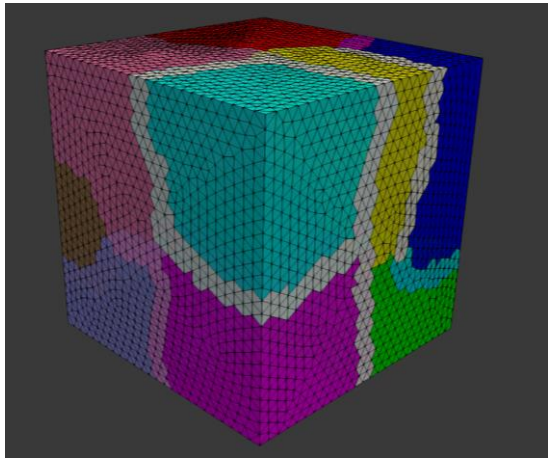
- Distributing the mesh among available resources
  - High-performance mesh decomposition
  - Overlapping Schwarz method
- Solving the linear system of equations
  - BoomerAMG preconditioner (for reaction-diffusion)
  - Fieldsplit preconditioner (for fluid flow)
  - GMRES iterative solver

High-performance Mesh Decomposition

- Mesh is decomposed using overlapping Schwarz preconditioner
- Each partition is assigned to one CPU core (MPI process)

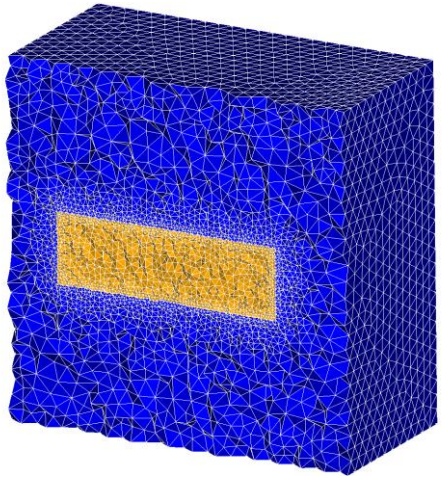


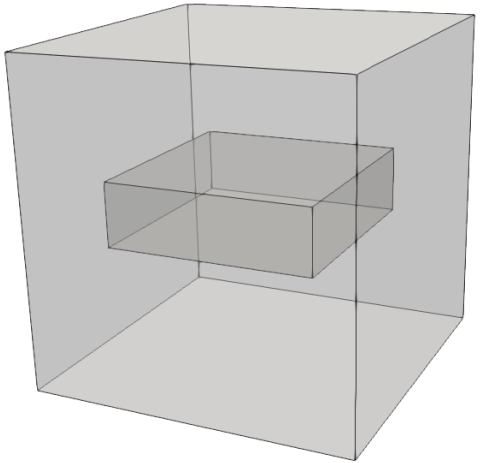




Performance Analysis

- A setup with a thick block
- Only 3 PDEs are solved
- DOF for each PDE ~ 150K
- Elements ~ 900K

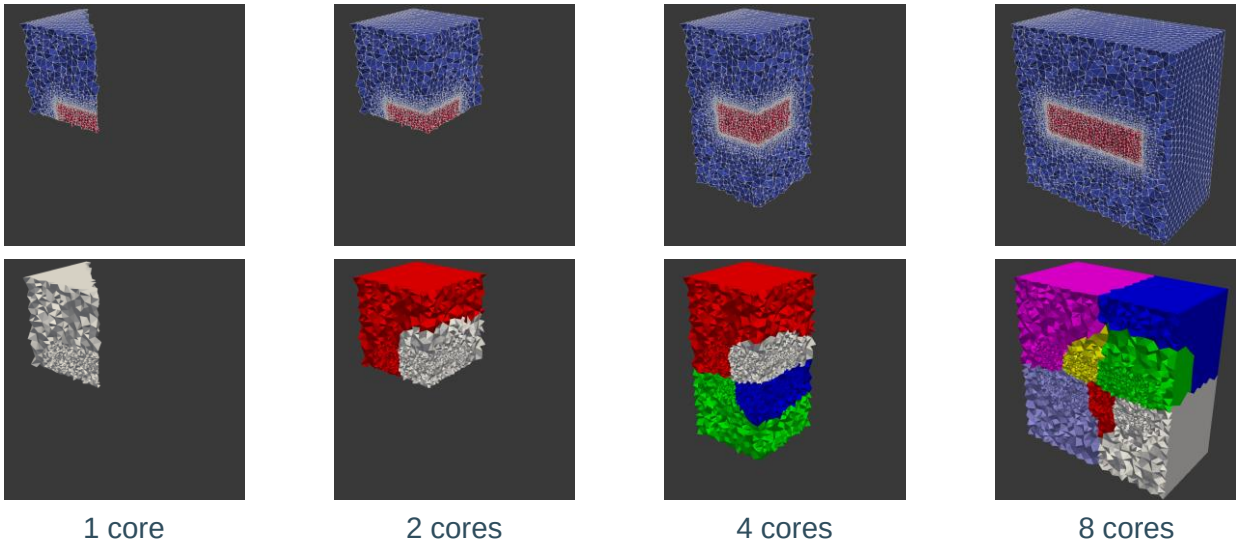




(Barzegari et al., Int. J. High. Perform. Comp., 35, 2021)

Parallelization Benchmark

- Weak scaling (doubling the problem size while doubling the resources)
- Strong scaling (keeping the problem size constant and doubling the resources)

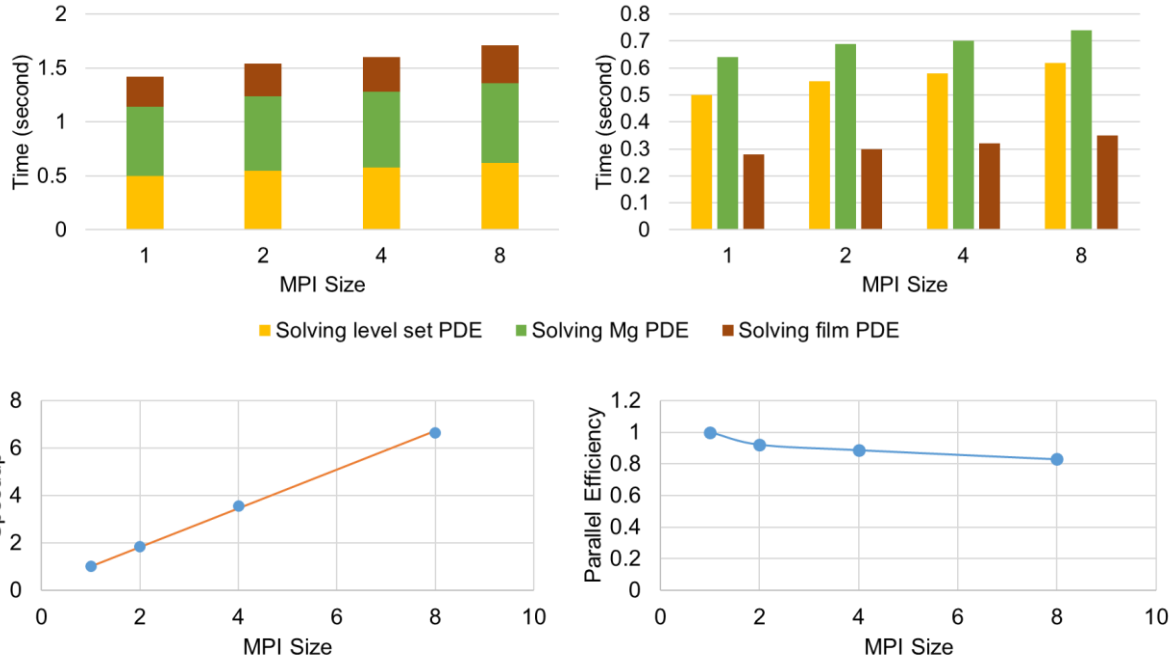


Weak Scaling Analysis

Gustafson's law

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

- Sequential part: 18%
- Parallel part: 82%



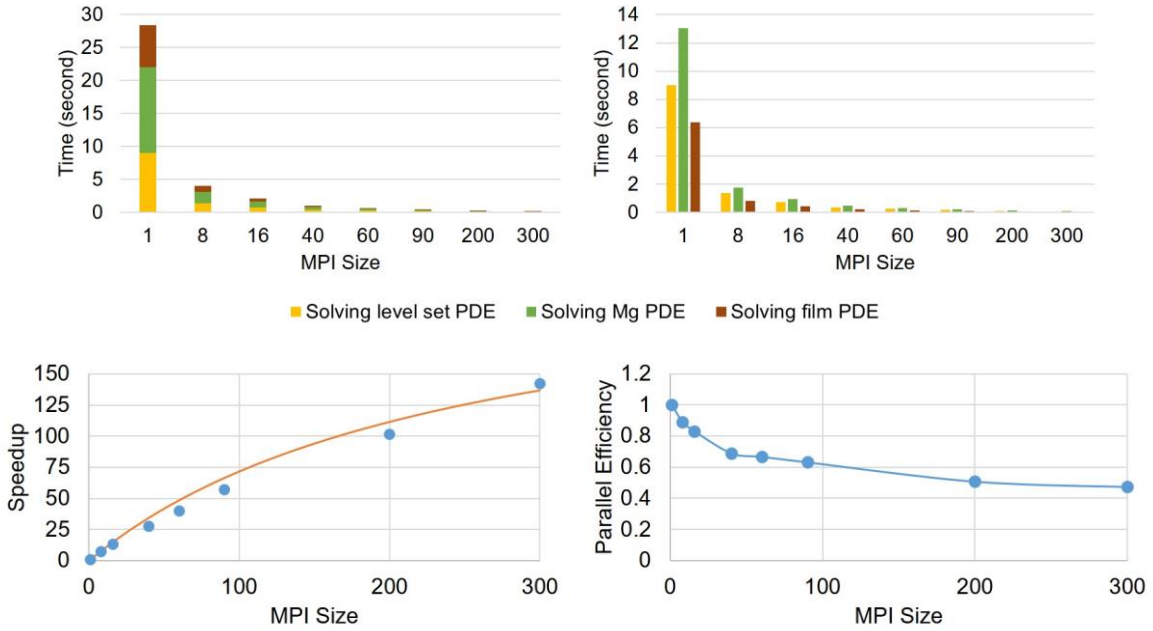
(Barzegari et al., Int. J. High. Perform. Comp., 35, 2021)

Strong Scaling Analysis

Amdahl's law

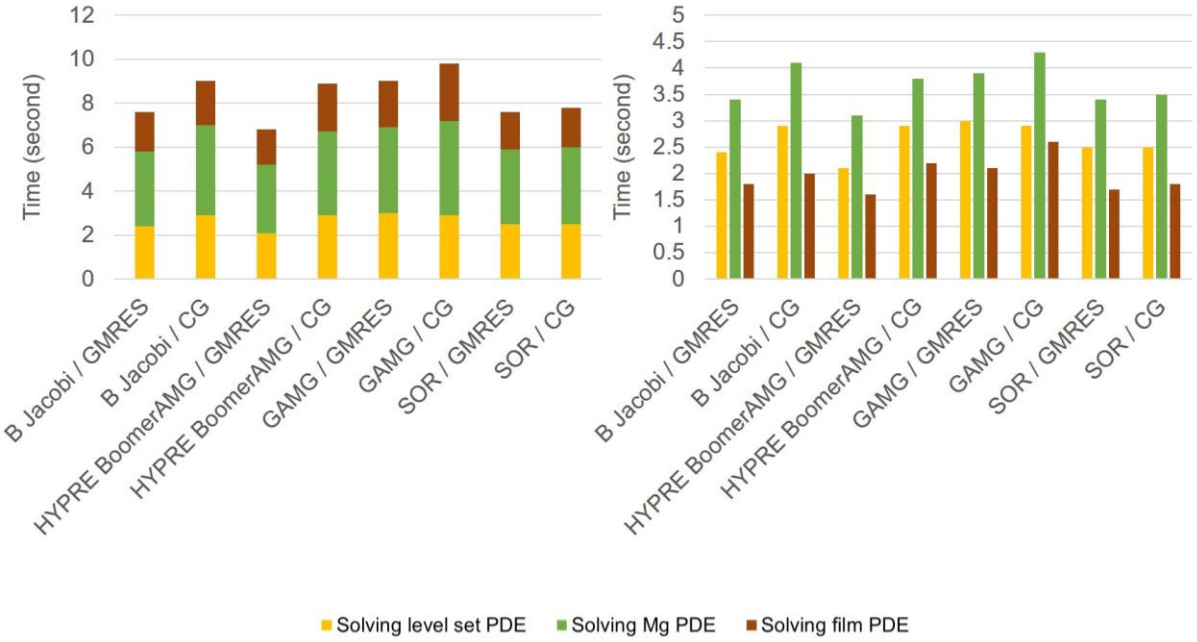
$$\text{Speedup} = \frac{1}{f + \frac{1-f}{N}}$$

- Sequential part: 1%
- Parallel part: 99%



(Barzegari et al., Int. J. High. Perform. Comp., 35, 2021)

Preconditioner/Solver Performance

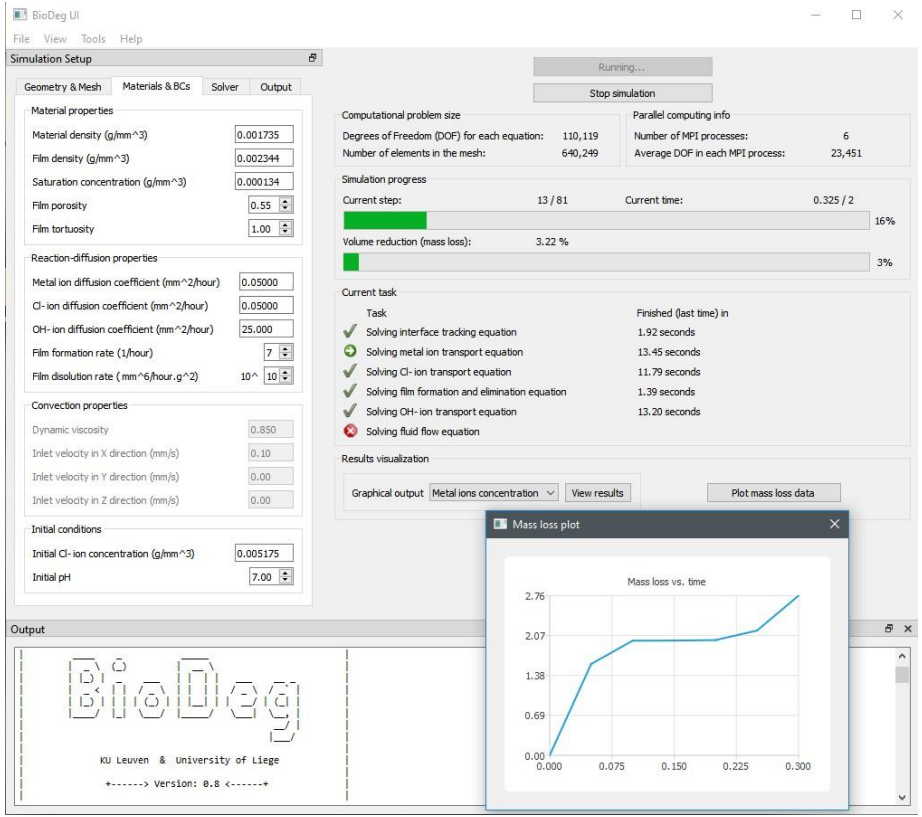


(Barzegari et al., Int. J. High. Perform. Comp., 35, 2021)

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



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)

User Interface

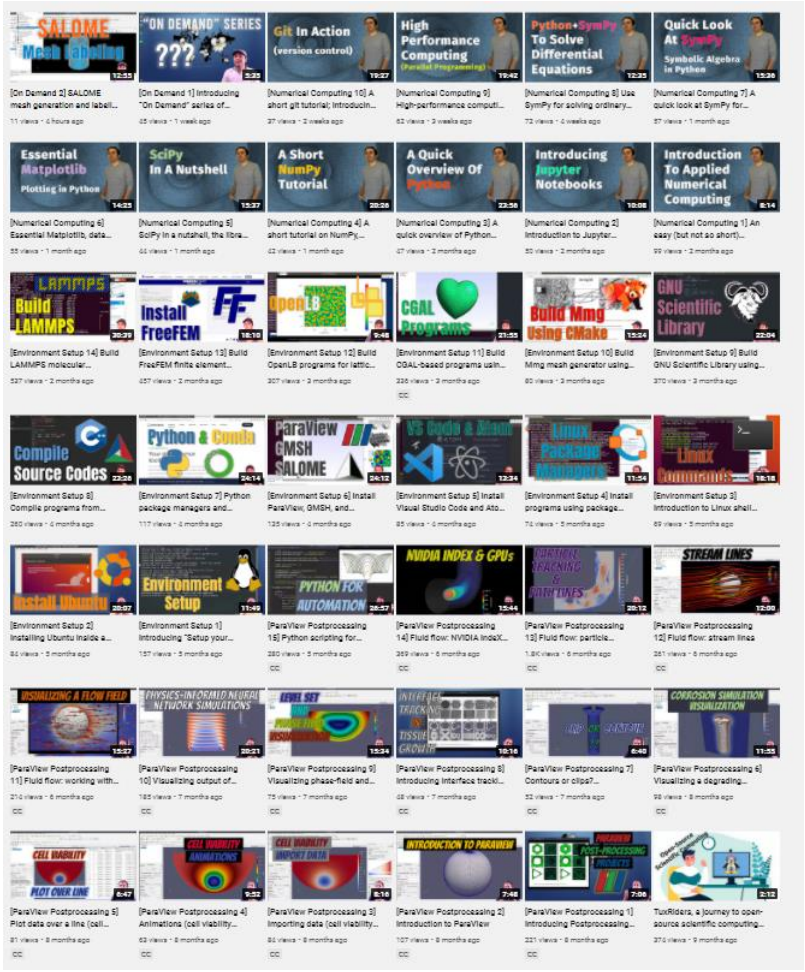
- Qt

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

A Final Note ☺

- A project to share experiences on scientific computing using open-source tools
- More info: TuxRiders.com
  YouTube.com/TuxRiders



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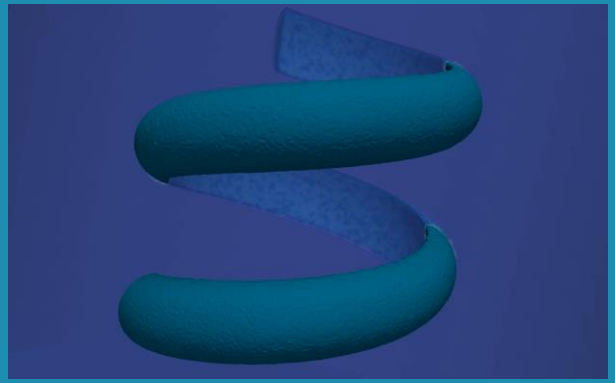

Thank you for your attention

https://mbarzegary.github.io

@MojBarz

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