High-performance computational modeling of metallic biomaterials biodegradation

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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

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 / Phase-field

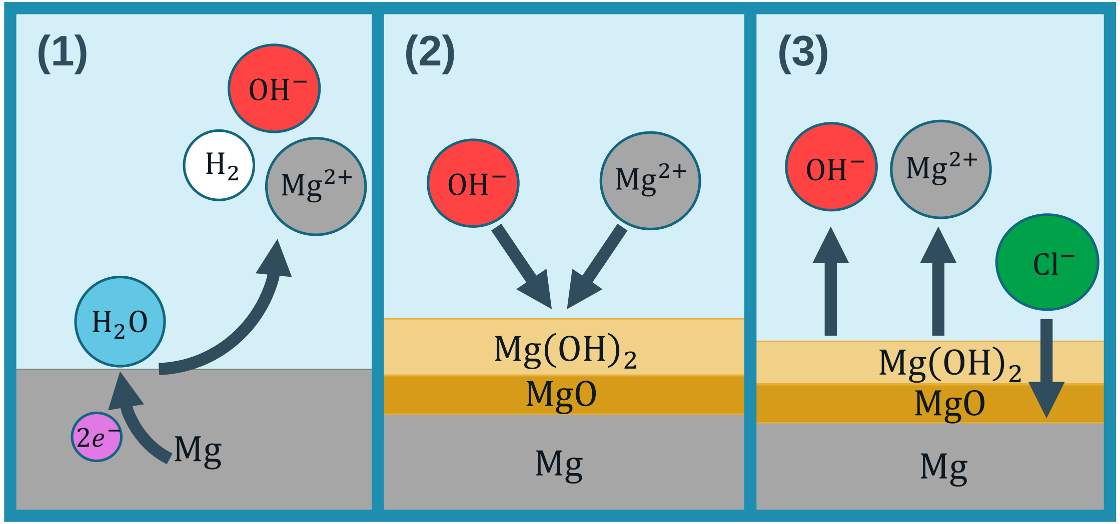
Computational Models
- Finite element method
- Finite difference method
- Parallel computing libraries
- Open source solvers

Computational Model of Biodegradation

Chemistry of Biodegradation

The model captures:

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



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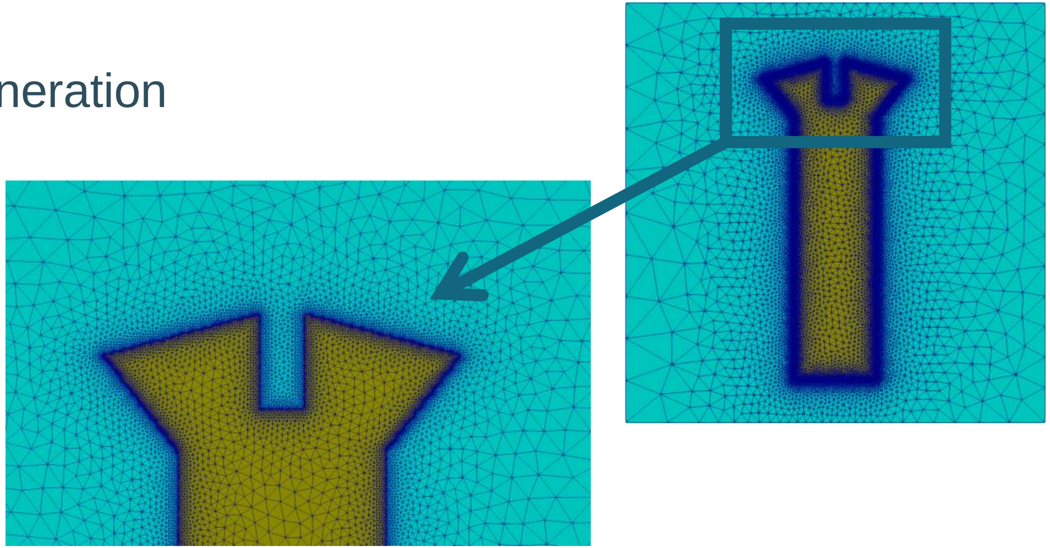
Constructing Mathematical Model

- Converting the chemical interactions 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

- Discretizing PDEs, finite element method
- Level-set for capturing the moving corrosion front
- Employing HPC techniques
- Adaptively refined mesh generation



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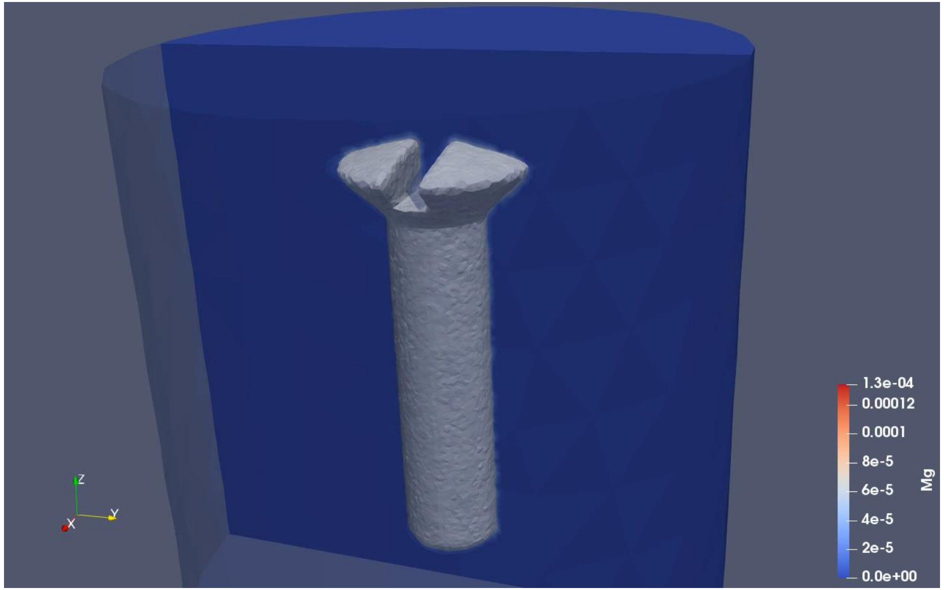
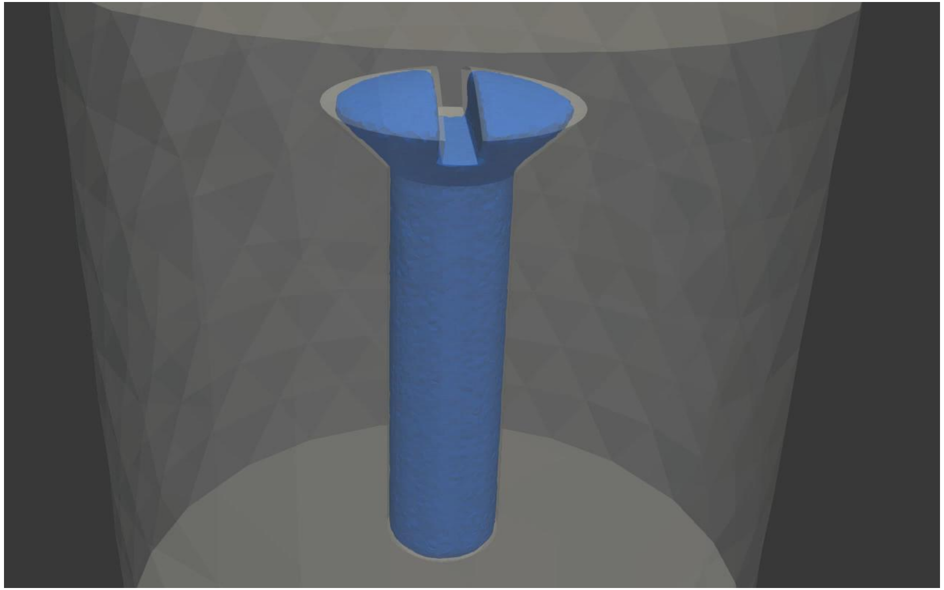
Simulation Results

Orthopedics Screw Degradation





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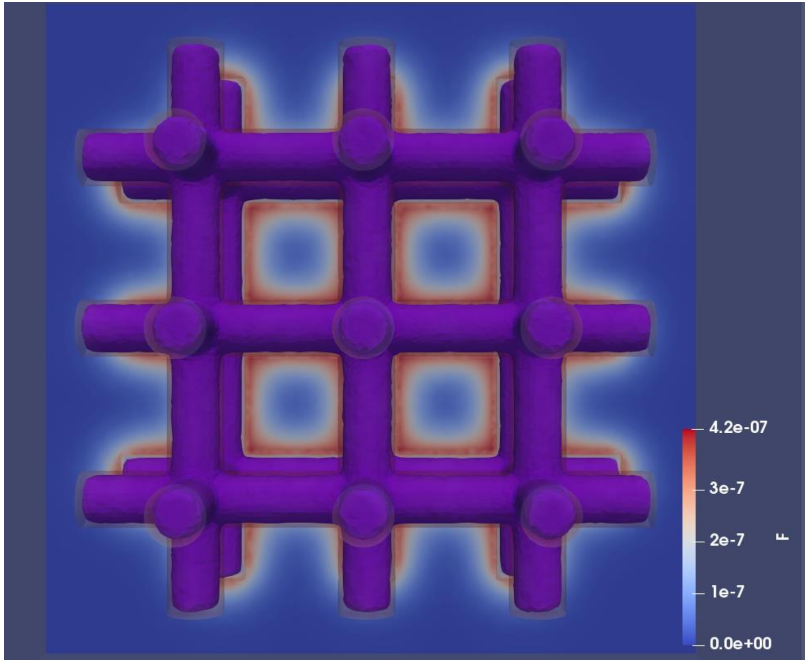
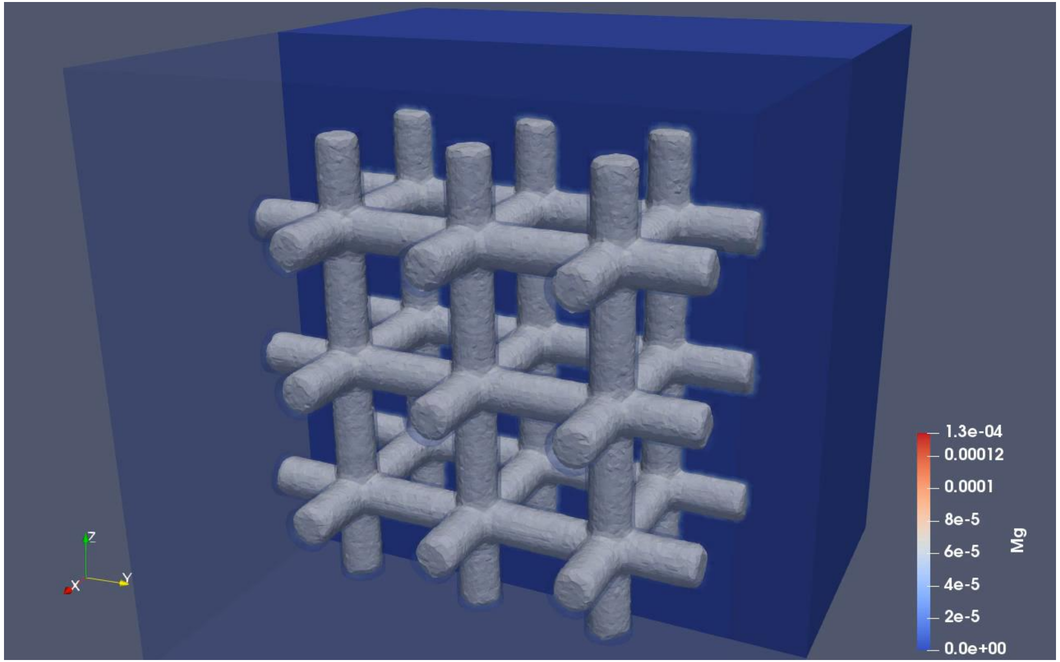
Porous Scaffold Degradation





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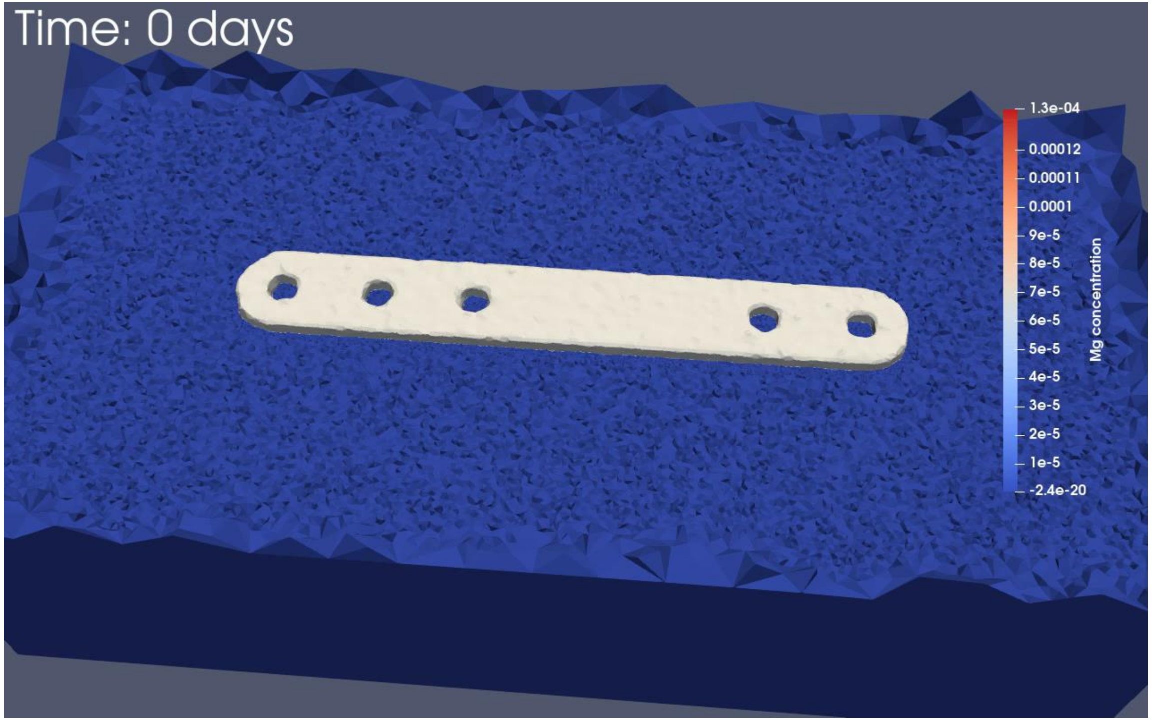
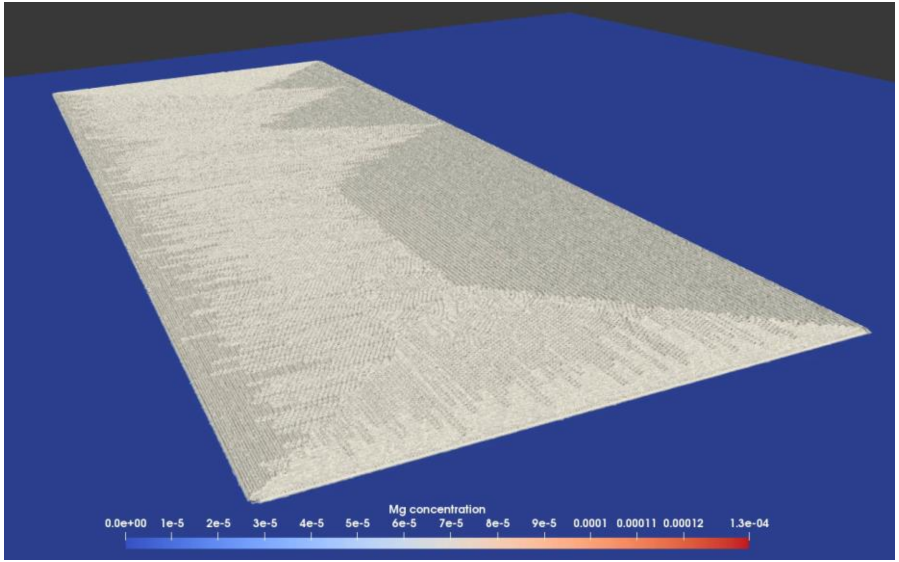
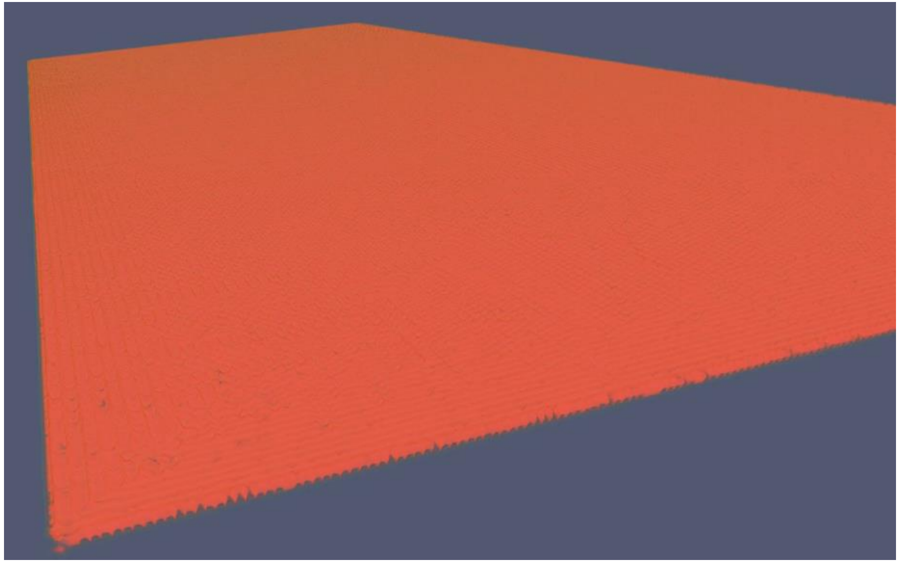
Jaw Bone Plate Degradation



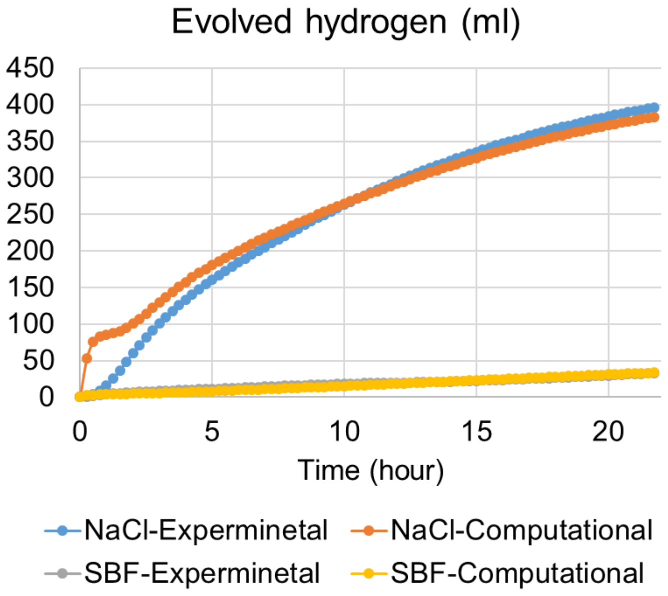
Narrow Cuboid

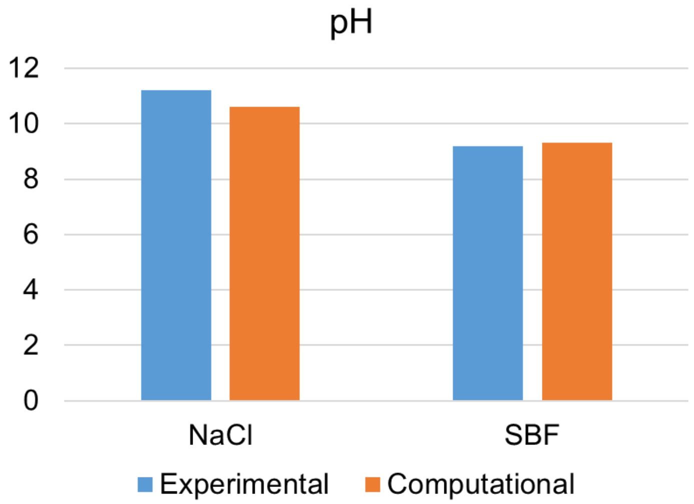




(Barzegari et al., Corrosion Science, 190, 2021)

Quantitative Results for Validation





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

Case Study:
Personalized Biodegradable Porous Acetabular Implants

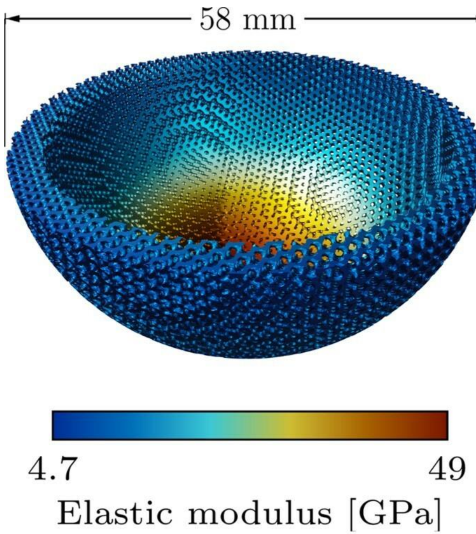
Bone Removal in Revision Surgeries

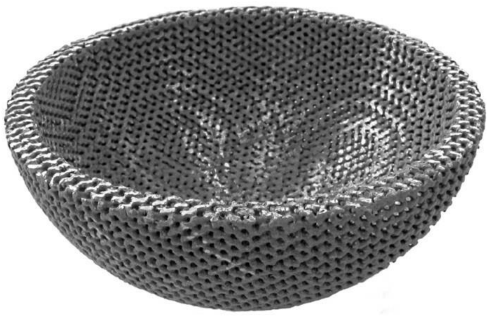
- Implants should be removed at the end of their lifetime
- Some extra bone is also removed along with the implant
- Making at least part of the implant from biodegradable materials

(Source: 3D Systems Inc.)

Optimized Acetabular Cup

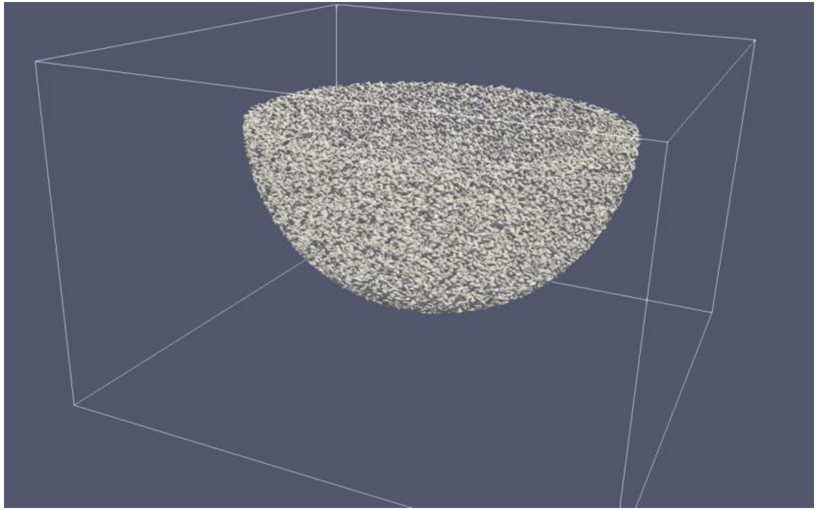
- Varying volume fraction to match a desired stiffness distribution
- Infilled with TPMS lattice structures

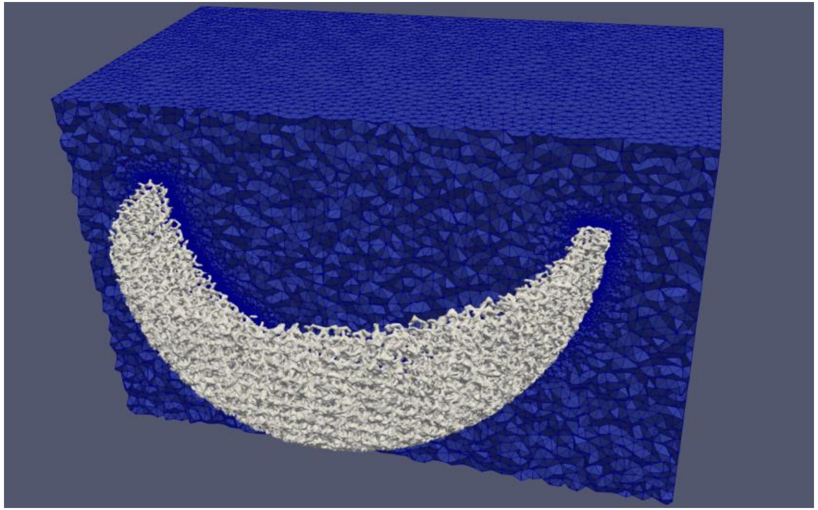




Simulation Setup

- Embedding the cup in a container and refine the mesh on its surface





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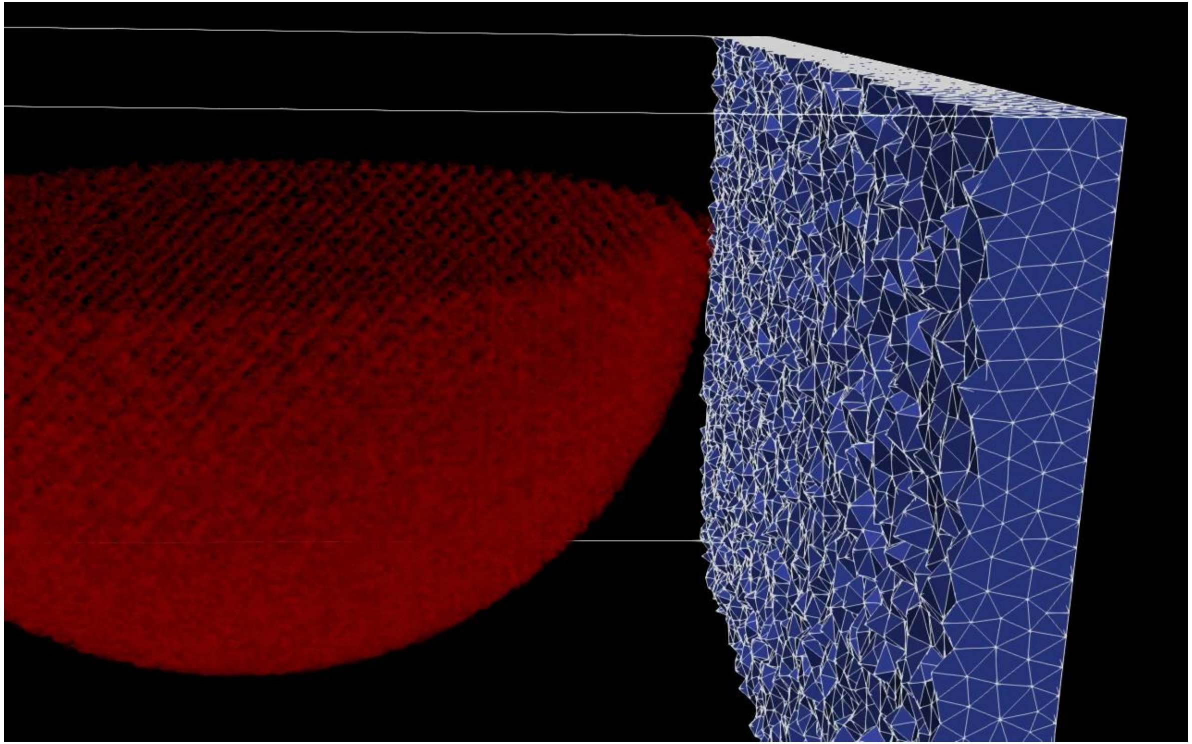
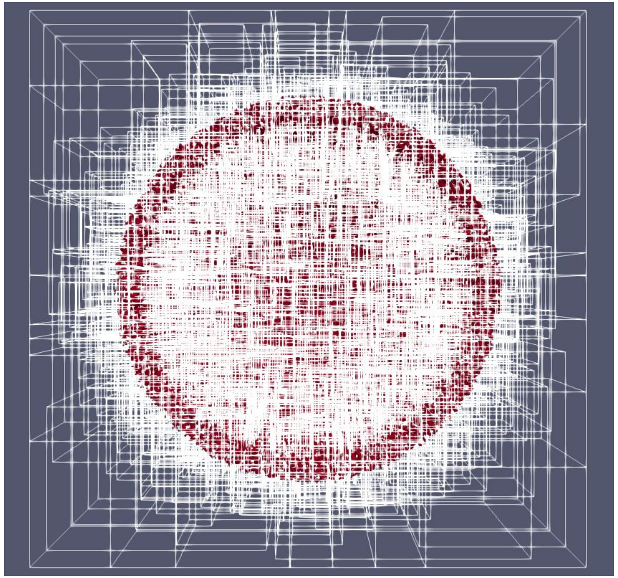
The Computational Mesh

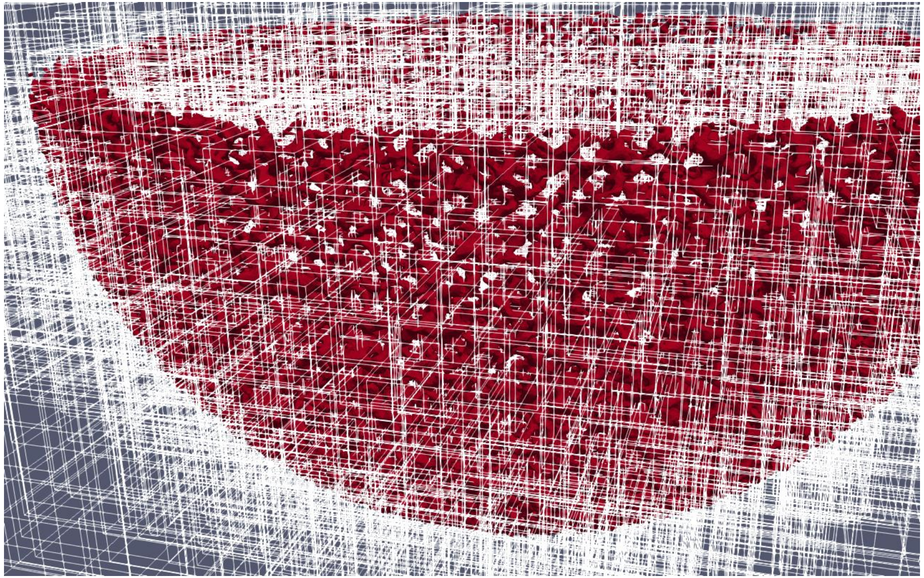
- Containing ~45M elements



Mesh Decomposition for HPC

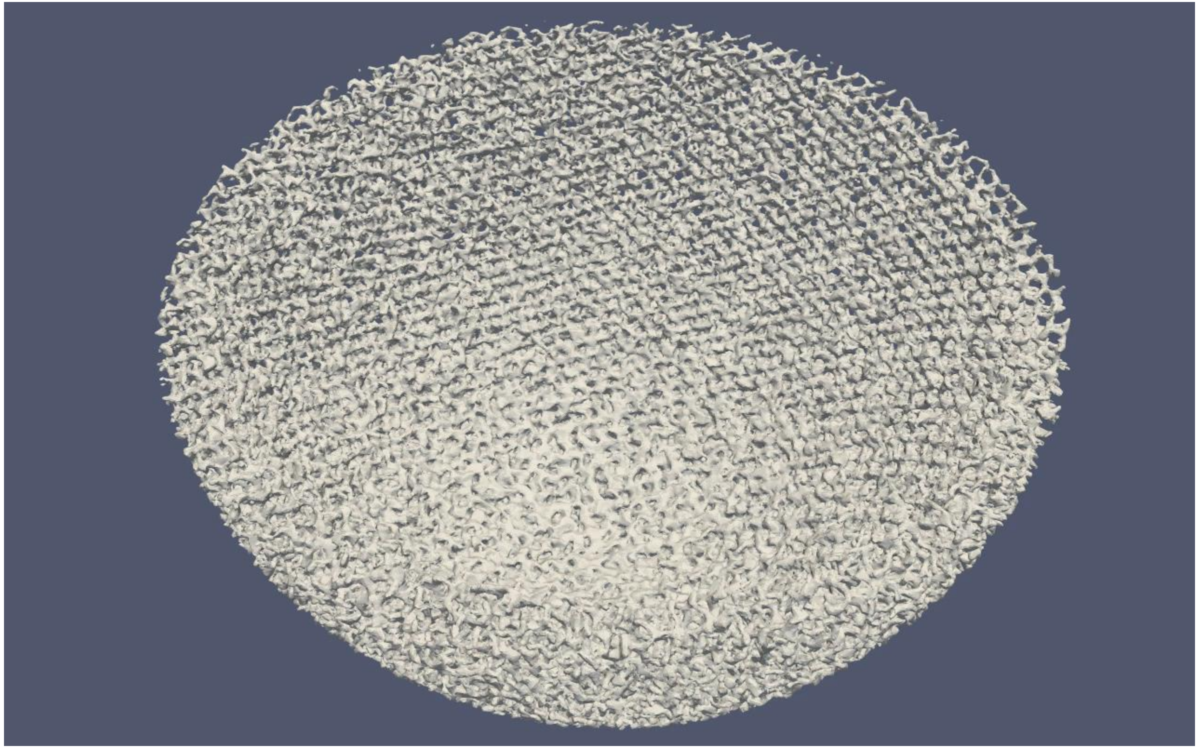
- Partitioning the mesh to be distributed to 2K - 8K CPU cores



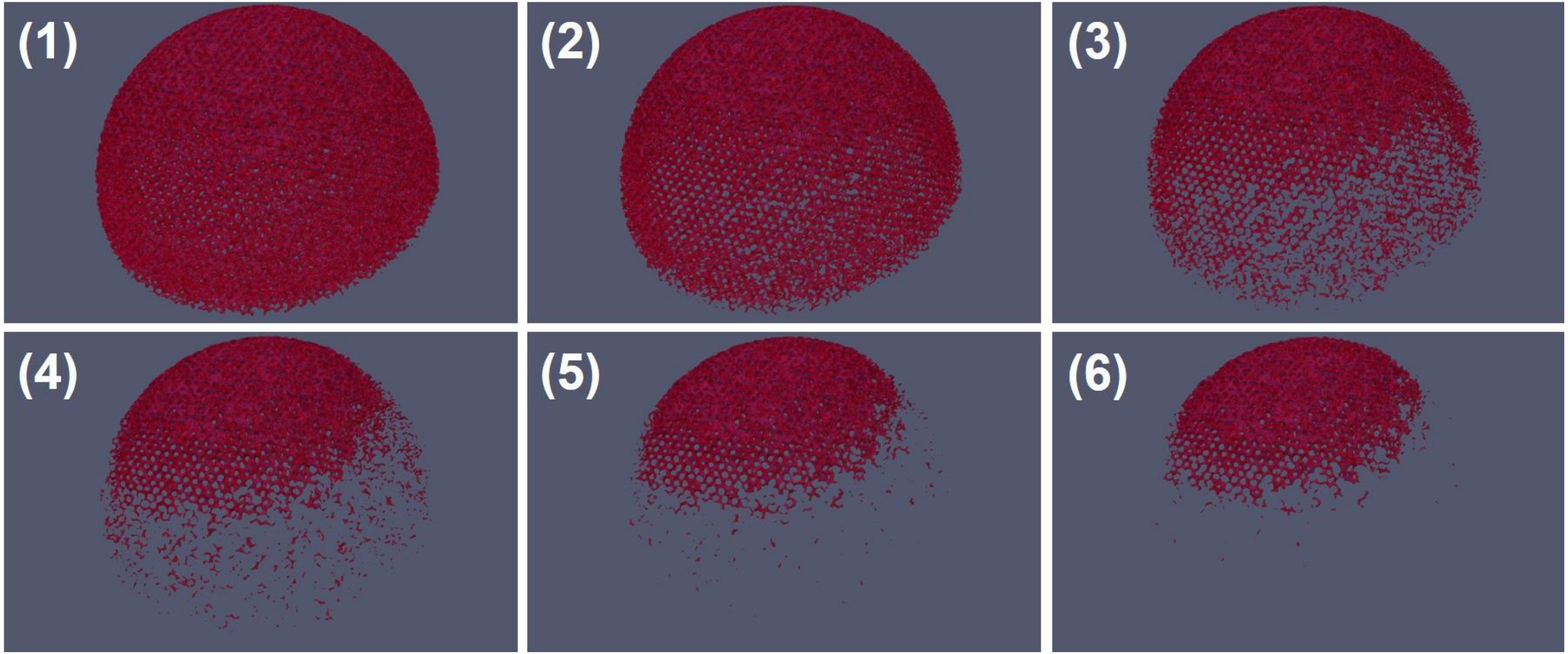


Degradation Behavior Result

- Visualization done using 128 CPU cores



Degradation Behavior Result



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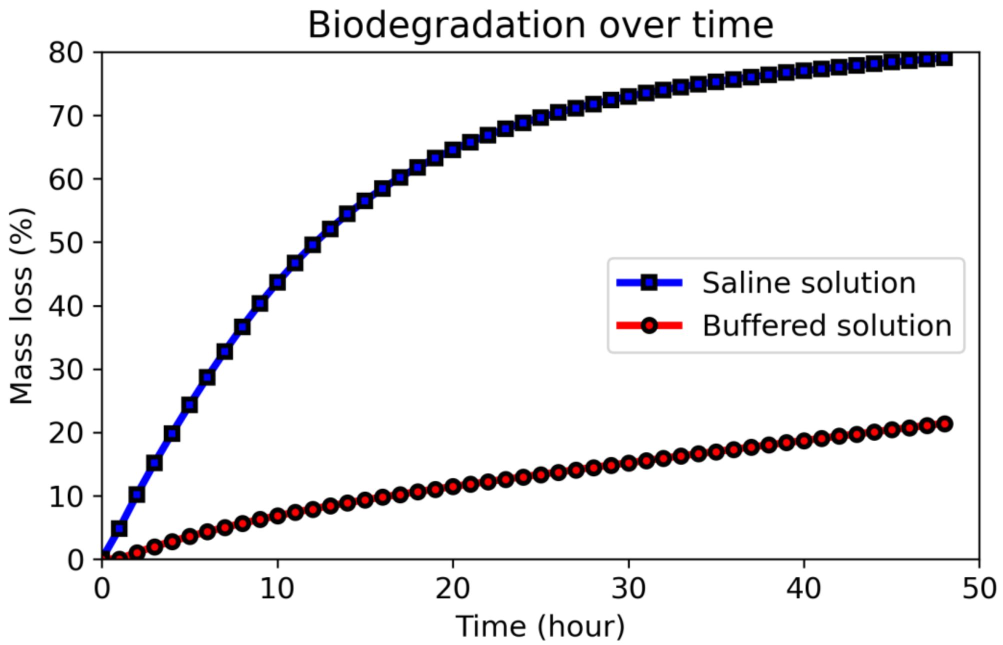
Degradation Rate Result



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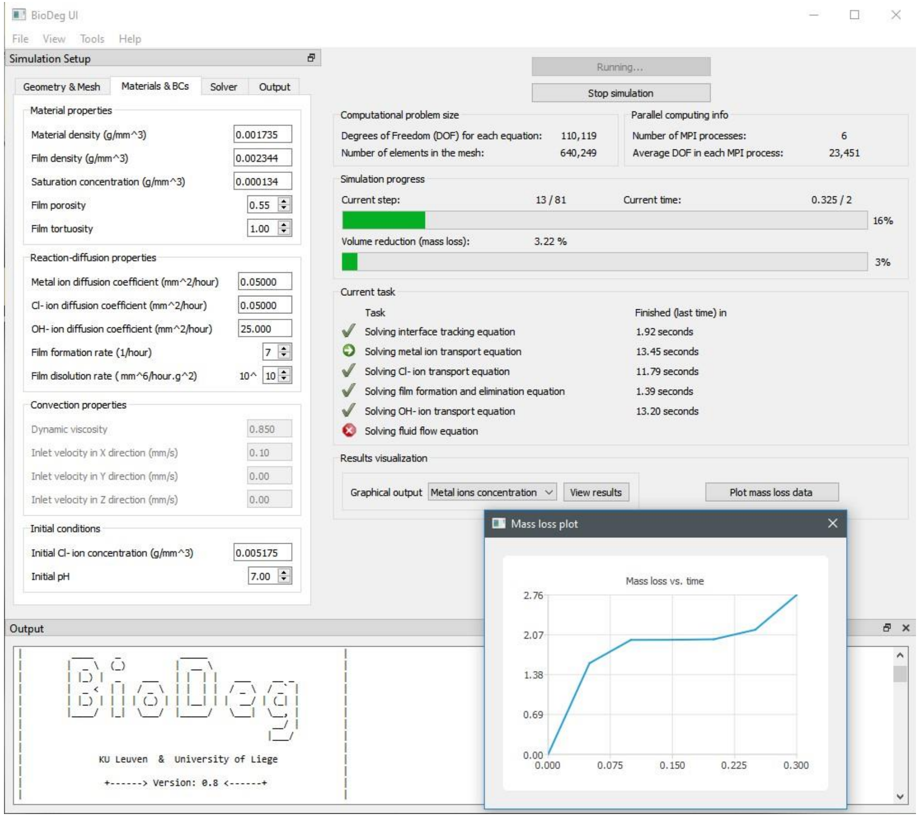
Software Development & Open-Source

BioDeg Software

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

https://github.com/mbarzegary/BioDeg-UI



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

https://github.com/mbarzegary

Acknowledgment

KU LEUVEN

- Prof. Liesbet Geris
- Fernando Perez-Boerema

UNIVERSITY OF AMSTERDAM

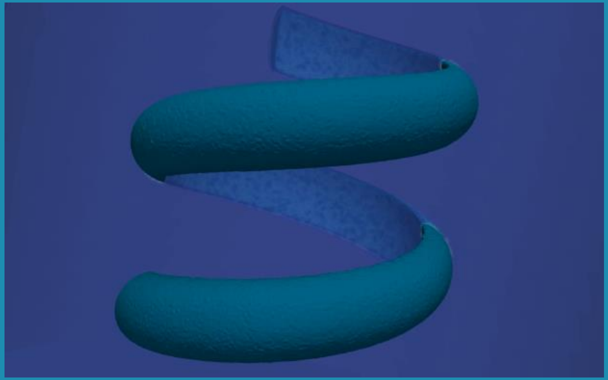
- Prof. Gabor Zavodszky

Helmholtz-Zentrum hereon

- Dr. Sviatlana Lamaka
- Dr. Di Mei
- Cheng Wang

prosperos

Interreg EUROPESE UNIE
Vlaanderen-Nederland
Europees Fonds voor Regionale Ontwikkeling



Thank you for your attention

https://mbarzegary.github.io

@MojBarz

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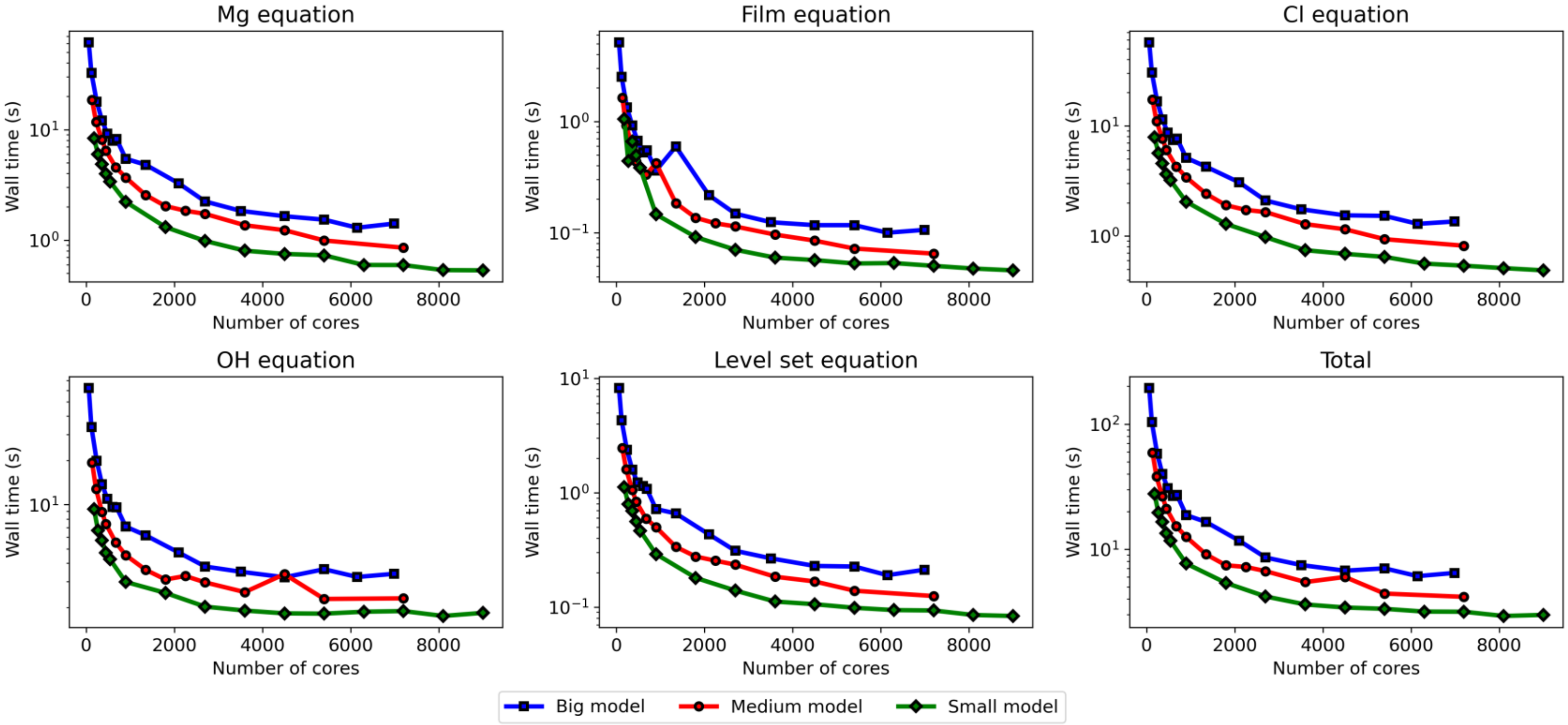
Strong Scaling Tests



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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)