

Four years of scientific computing using FreeFEM in the field of computational biomedical engineering

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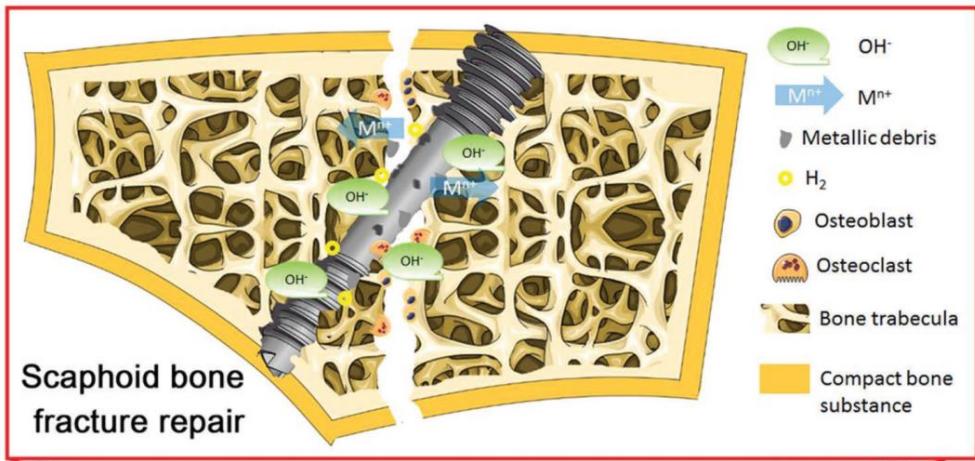
FreeFEM in Biomedical Engineering

- Computational biomechanics research unit (<http://www.biomech.ulg.ac.be/>)
- A wide range of models of tissue engineering processes
- FreeFEM benefited us due to:
 - Freedom in controlling finite element spaces
 - Open standards / exchange formats / interoperability
 - Integration with other tools
(PETSc, HPDDM, Mmg, Tetgen, METIS, etc.)

Computational modeling of biodegradation process of metallic biomaterials

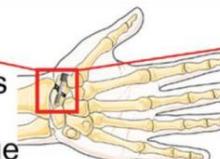
Biodegradable Metals

- Dissolve upon fulfilling the mission to assist tissue healing
- The degradation behavior should be tuned/optimized
- A set of reaction-diffusion-advection PDEs describing the chemistry of biodegradation
- Level-set for tracking the moving corrosion front



Scaphoid bone
fracture repair

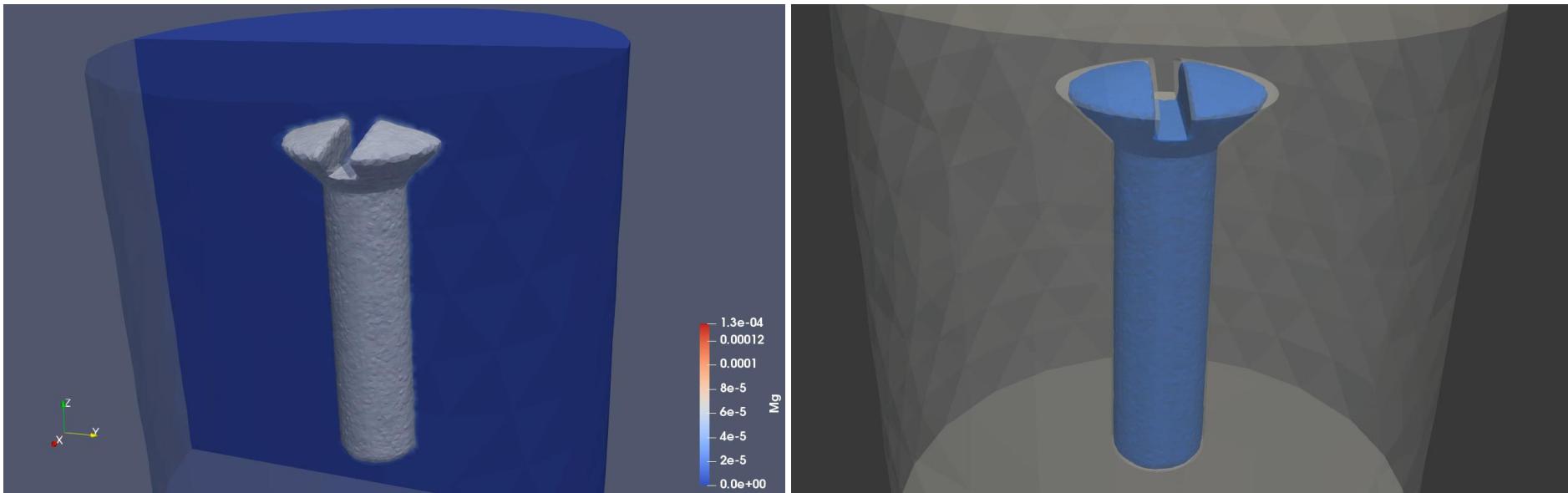
Absorbable:
Biodegradation products
are metabolized or
assimilated by cells/tissue



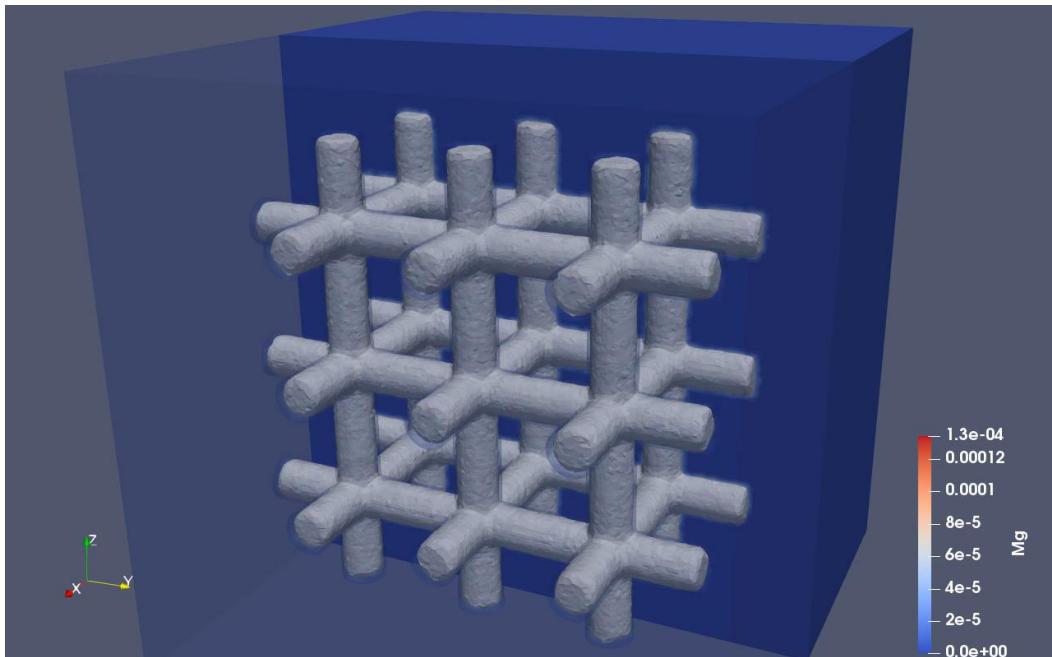
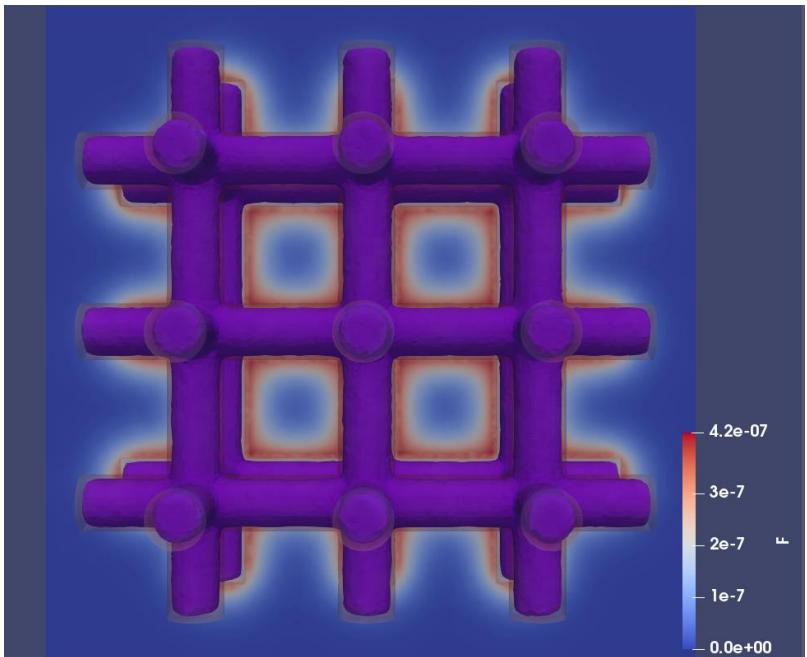
Biodegradable:
The material/device itself
undergoes
biodegradation process

(Liu et al., Adv. Funct. Mater., 29, 2019)

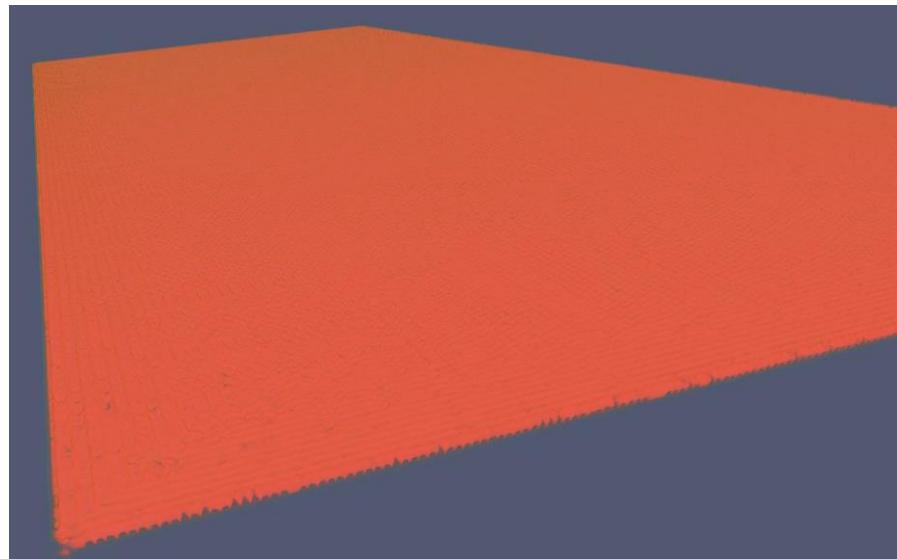
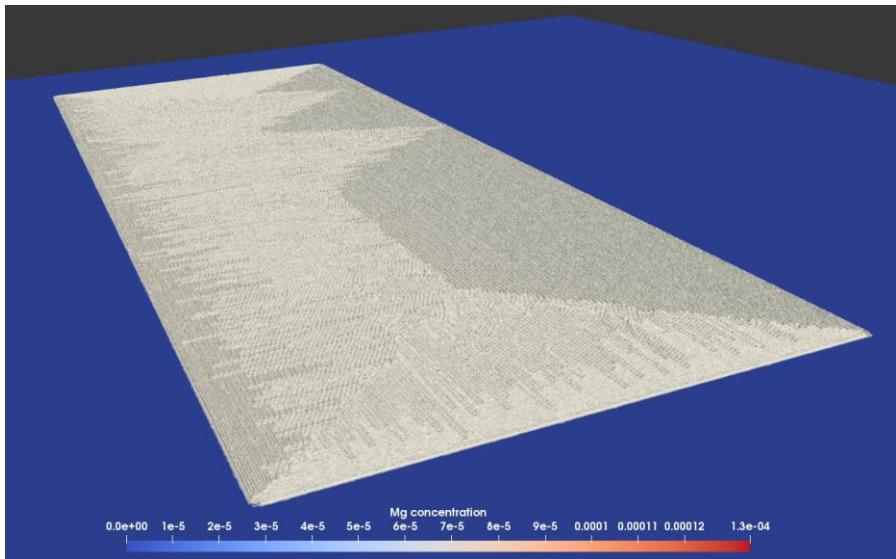
Orthopedics Screw Degradation



Porous Scaffold Degradation



Narrow Cuboid



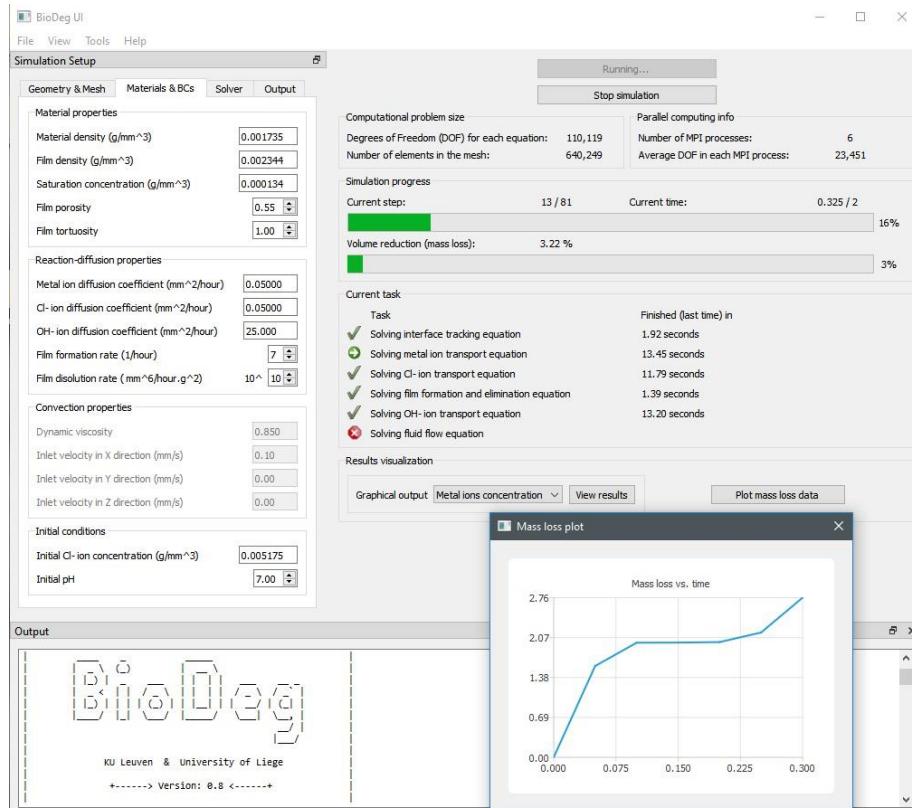
(Barzegari et al., Corrosion Science, 190, 2021)

BioDeg Software

- Multifunctional parallel 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

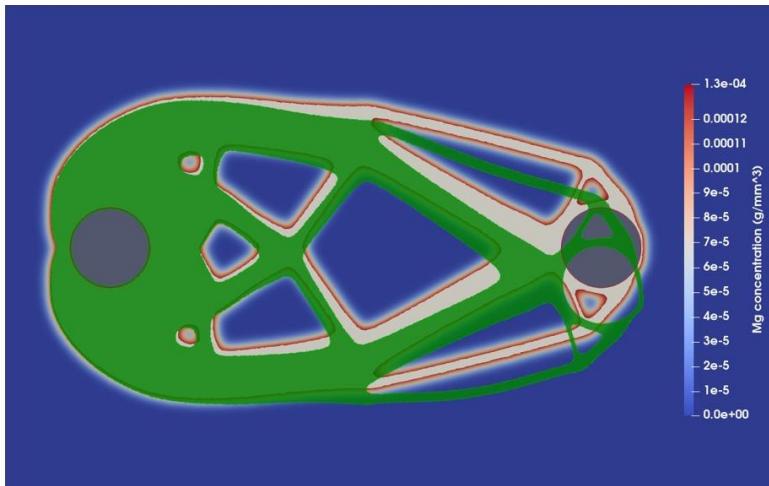
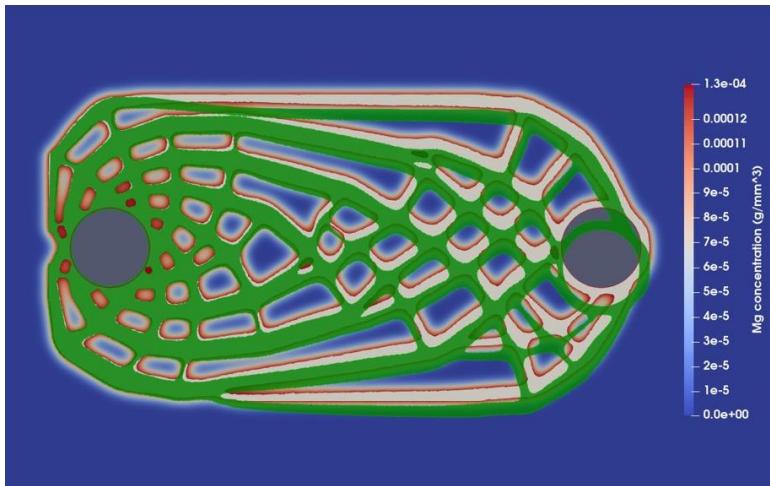


<https://github.com/mbarzegary/BioDeg-UI>



Model Integration

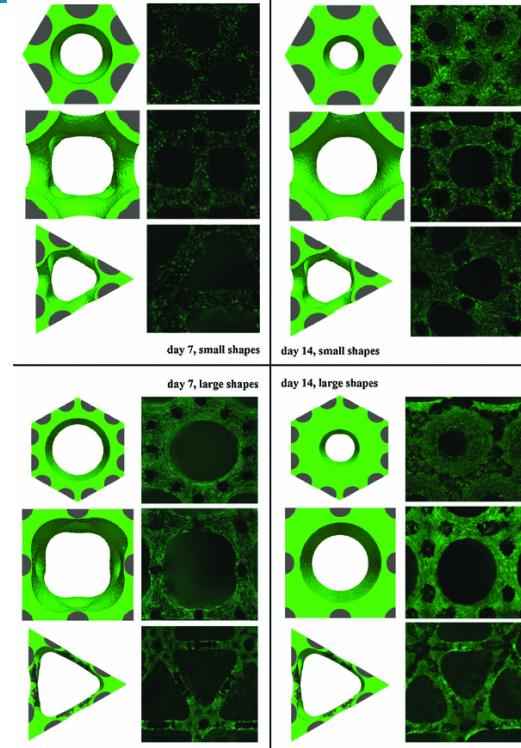
- Coupled models of topology optimization and metals corrosion for optimizing the shape of biodegradable infilled structures



Computational modeling of tissue regeneration and growth

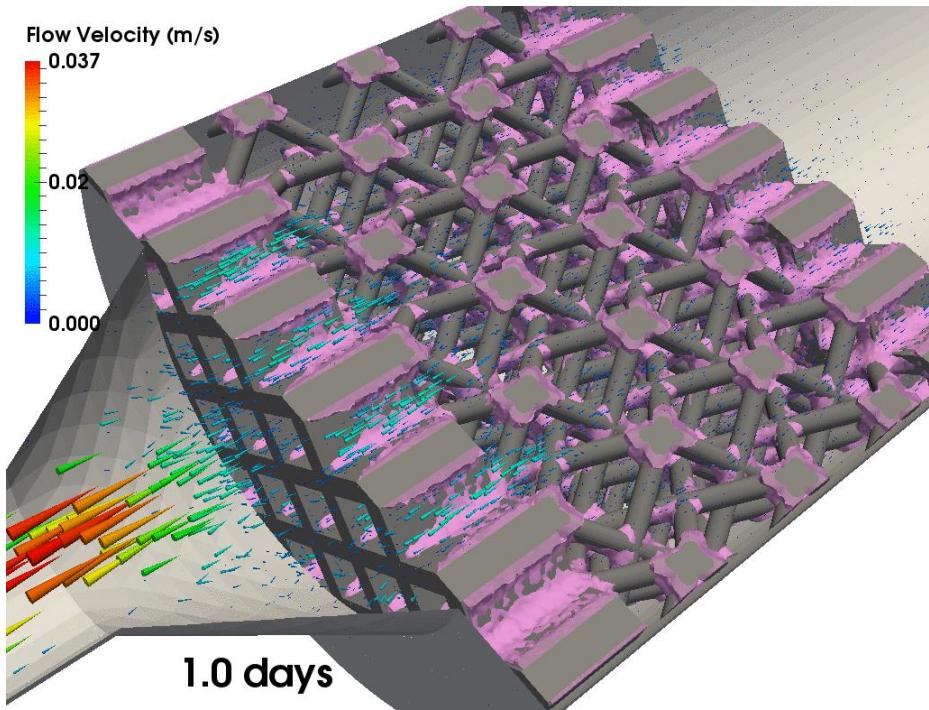
Curvature-based Tissue Growth

- Cell growth on open porous scaffolds
- Effect of geometrical characteristics (pore size, shape, and curvature)
- Computational models of tissue regeneration process
- Modeling growth as a moving interface problem:
 - Level-set method
 - Phase-field method

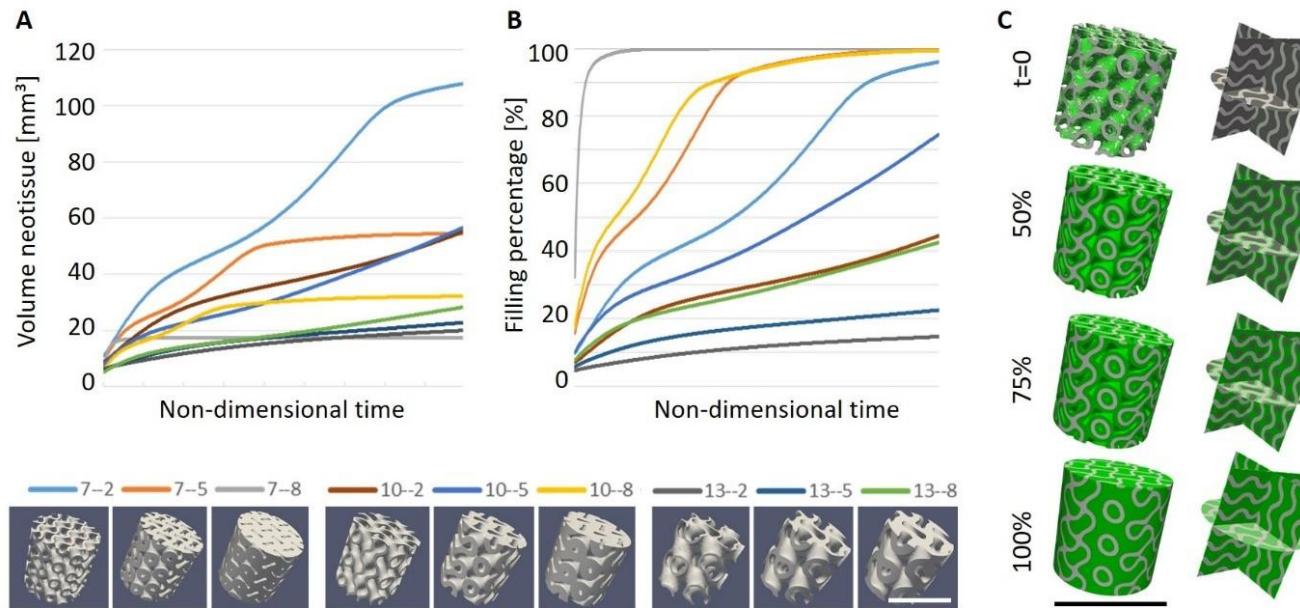


(Guyot et al., Biomech Model Mechanobiol., 13, 2014)

Tissue Regeneration in Bioreactors

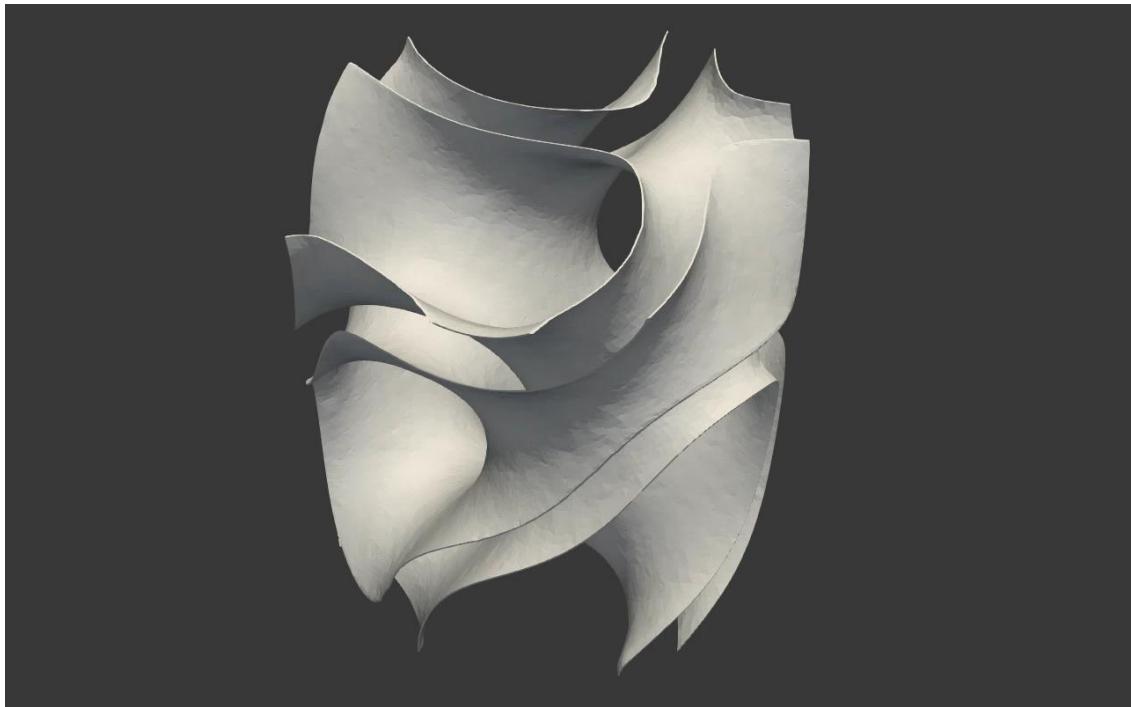
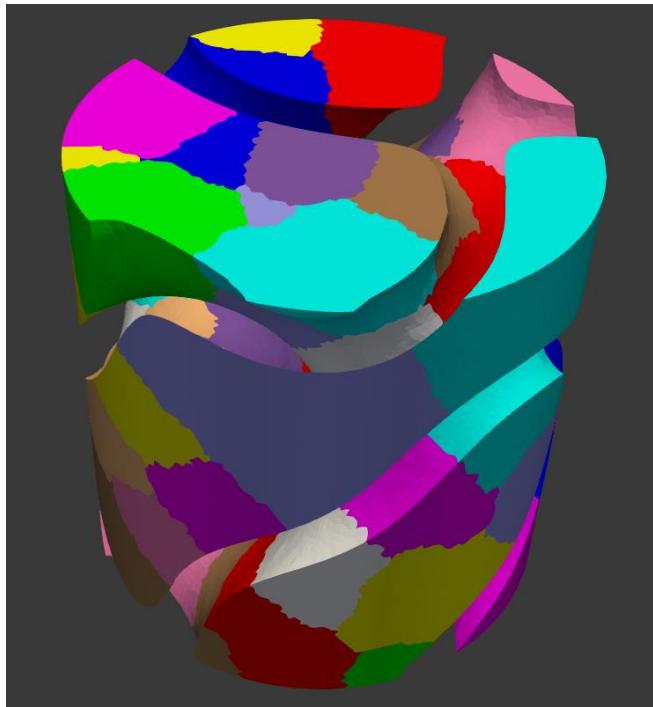


Tissue Growth on Various Scaffolds



(Van Hede et al., Adv. Funct. Mater., 32, 2022)

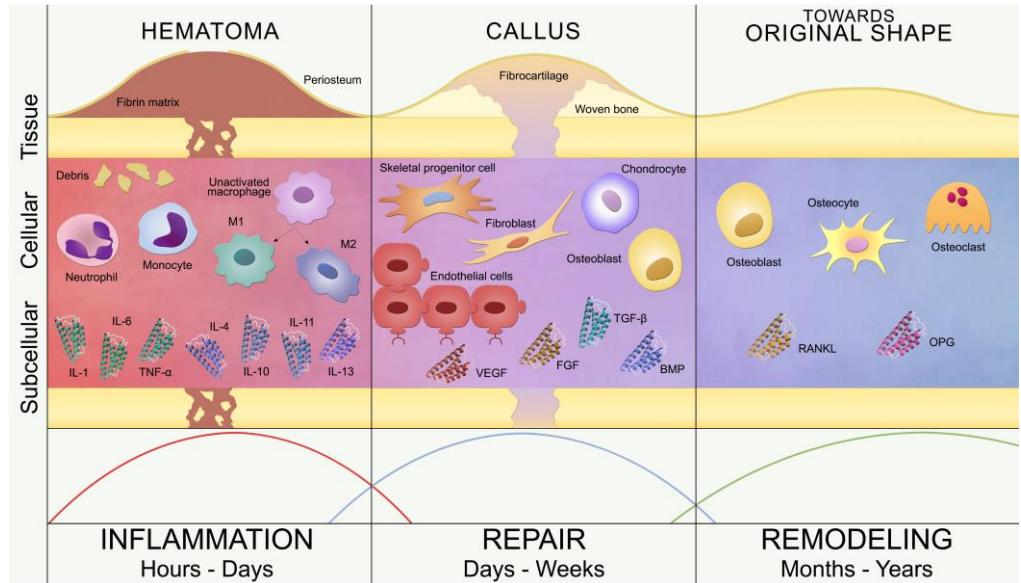
Parallel Implementation of Interface Tracking



Computational modeling of bone fracture healing

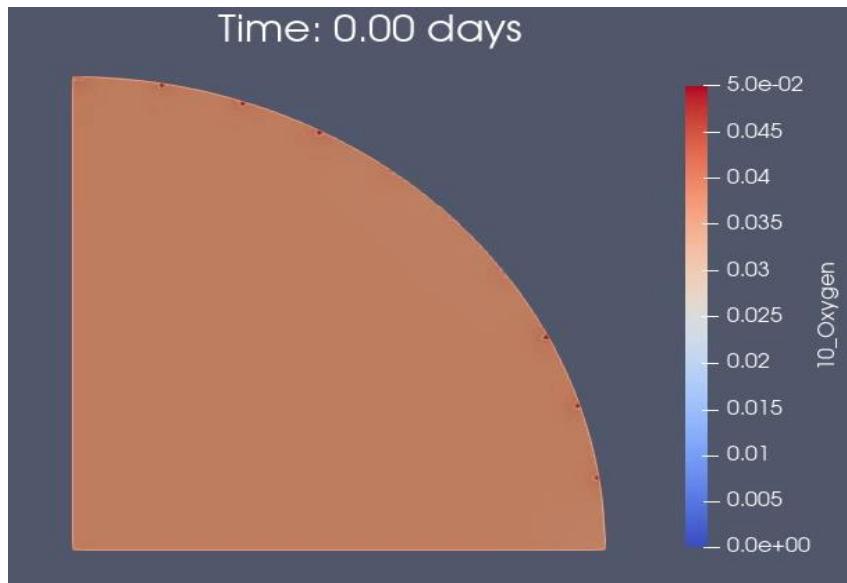
Repair Phase of Healing Process

- Bone fracture healing models to simulate the repair phase
- A set of taxis-diffusion-reaction PDEs for the evolution of cells, biochemical factors, and tissues
- Coupled with a cellular automaton model of blood vessels growth

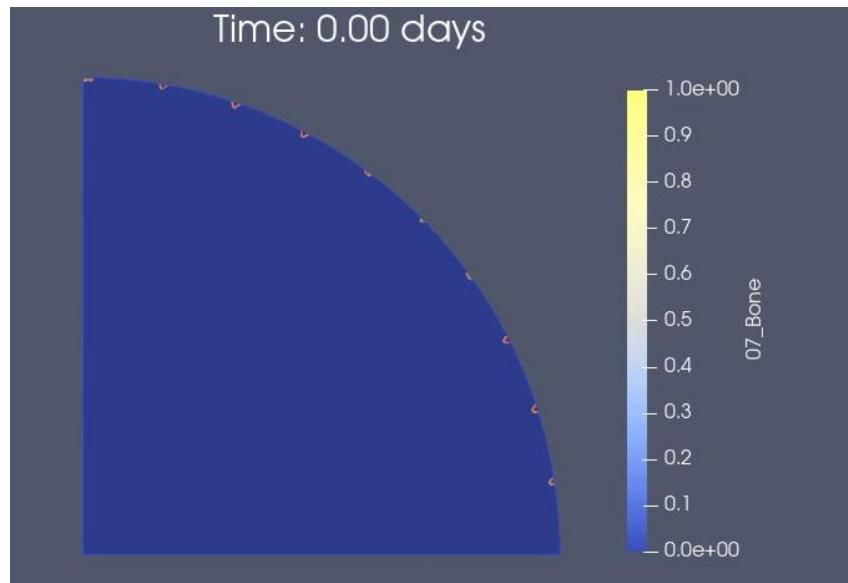


(Lafuente-Gracia et al., Front. Bioeng. Biotechnol, 2021)

Bone Regeneration for Mandibular Defects

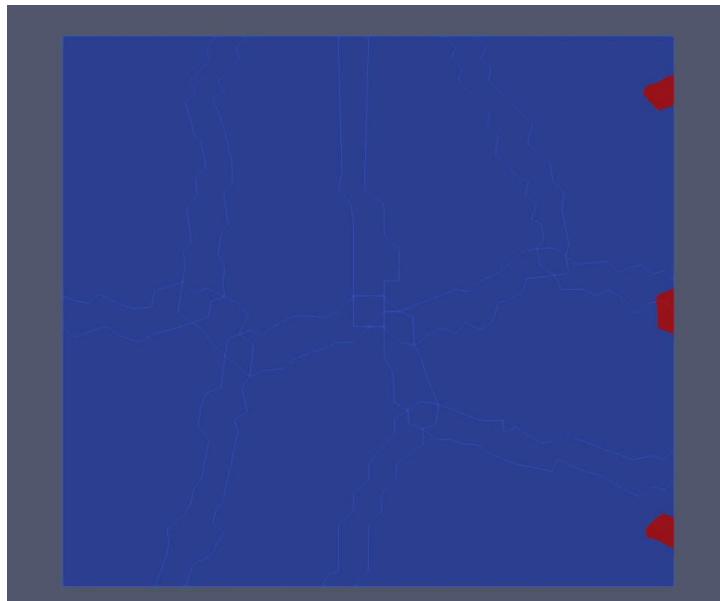


Vascular network & oxygen supply

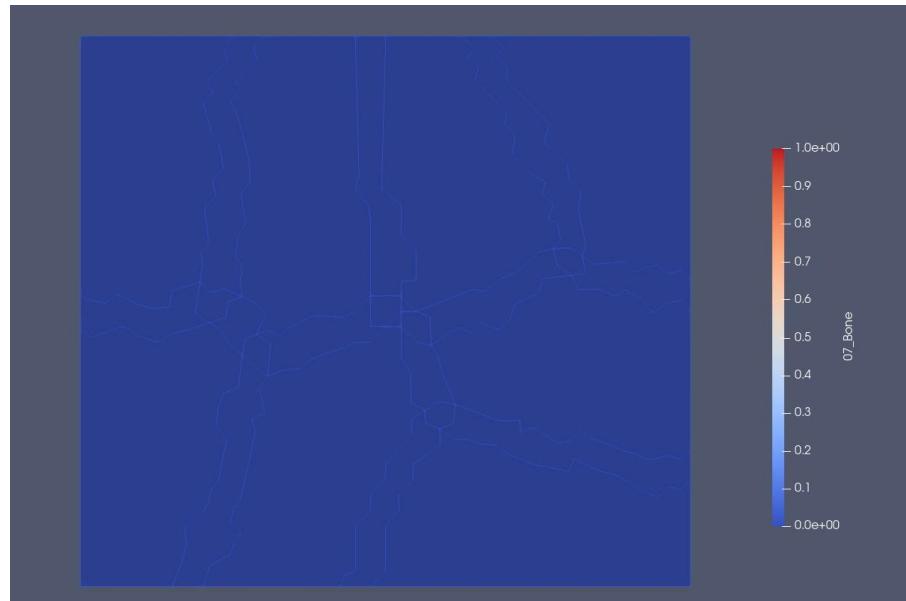


Bone formation

Parallelized Coupled FE-CA Model



Vessels growth



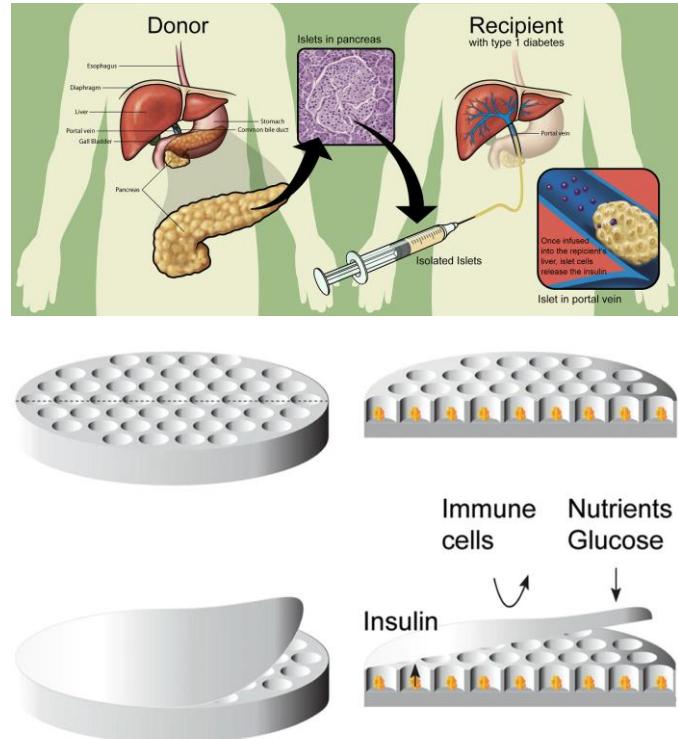
Bone formation

Computational modeling of pancreatic cells viability

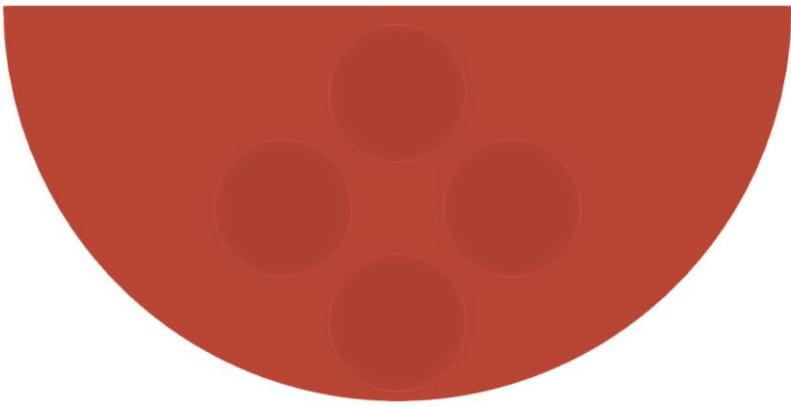
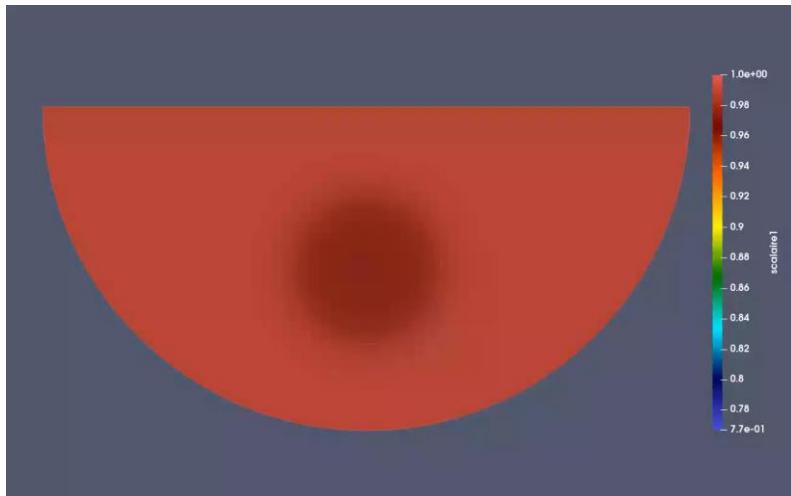
Pancreatic Cells Transplantation

- Islet transplantation to treat type 1 diabetes
- Vulnerability of cultured pancreatic islets
- Putting islets into micro-devices inside wells for gradient-driven oxygen supply
- Reaction-diffusion model for assessing viability of cells

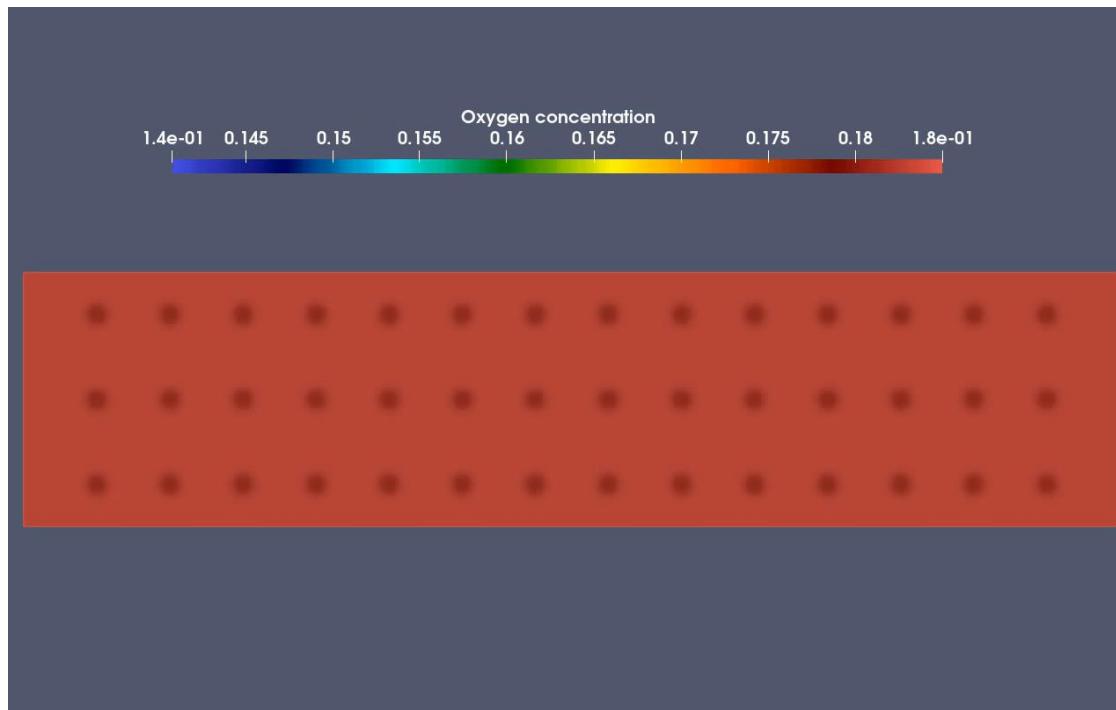
(sources: M.A. Naftanel et al., 2004, and K. Skrzypek et al., 2017)



Single Micro-device Simulations



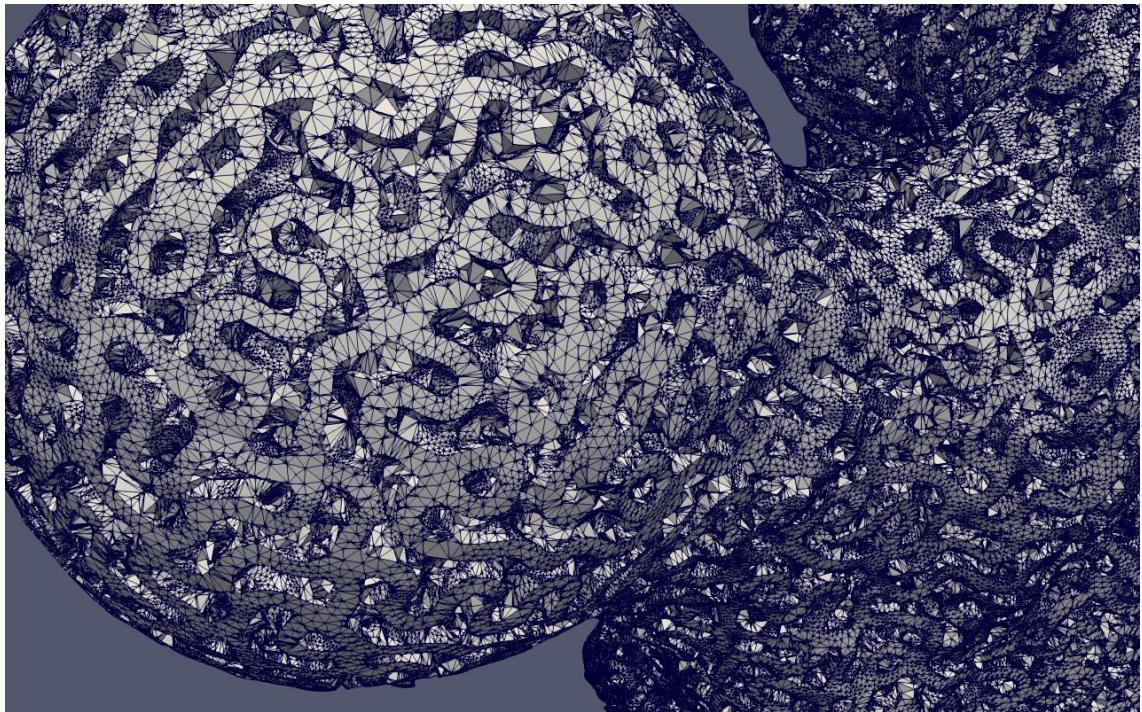
Islets Group, Multiple Wells



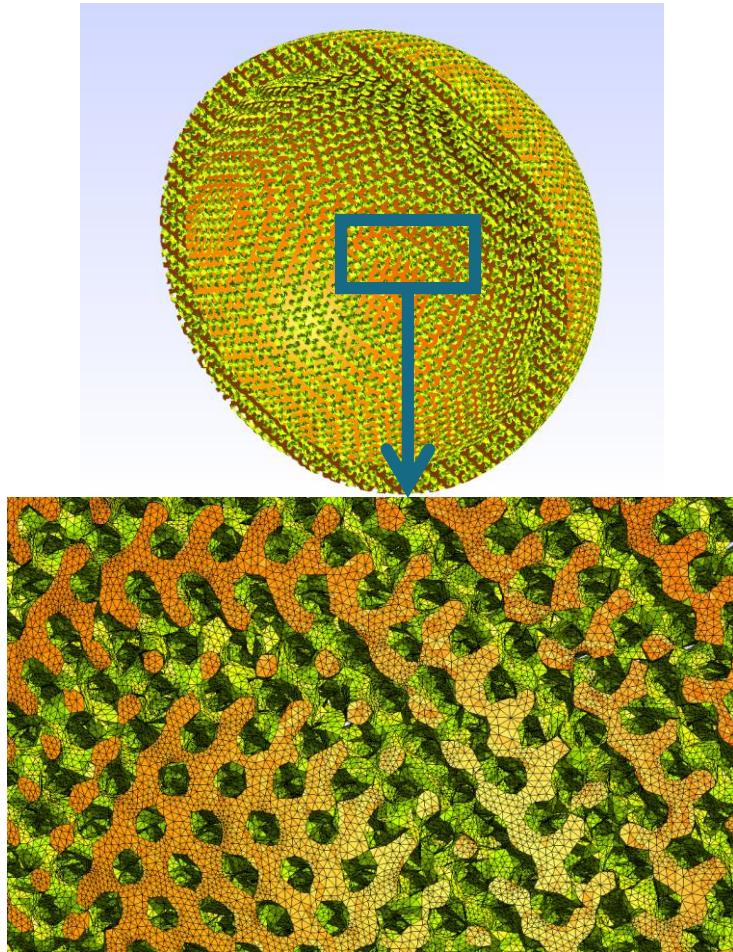
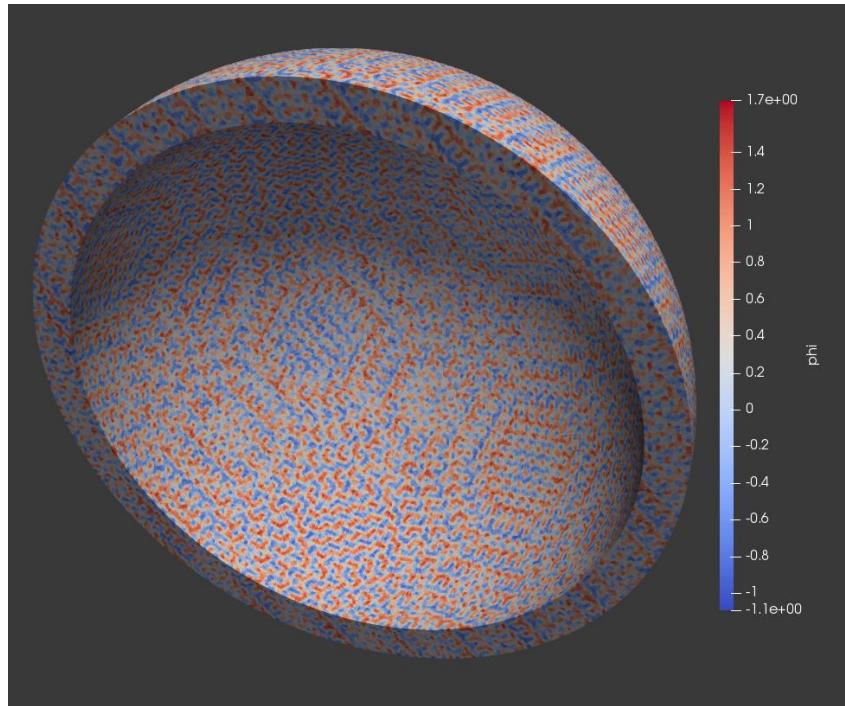
Geometry construction and mesh generation

Implicit Mesh Constructions

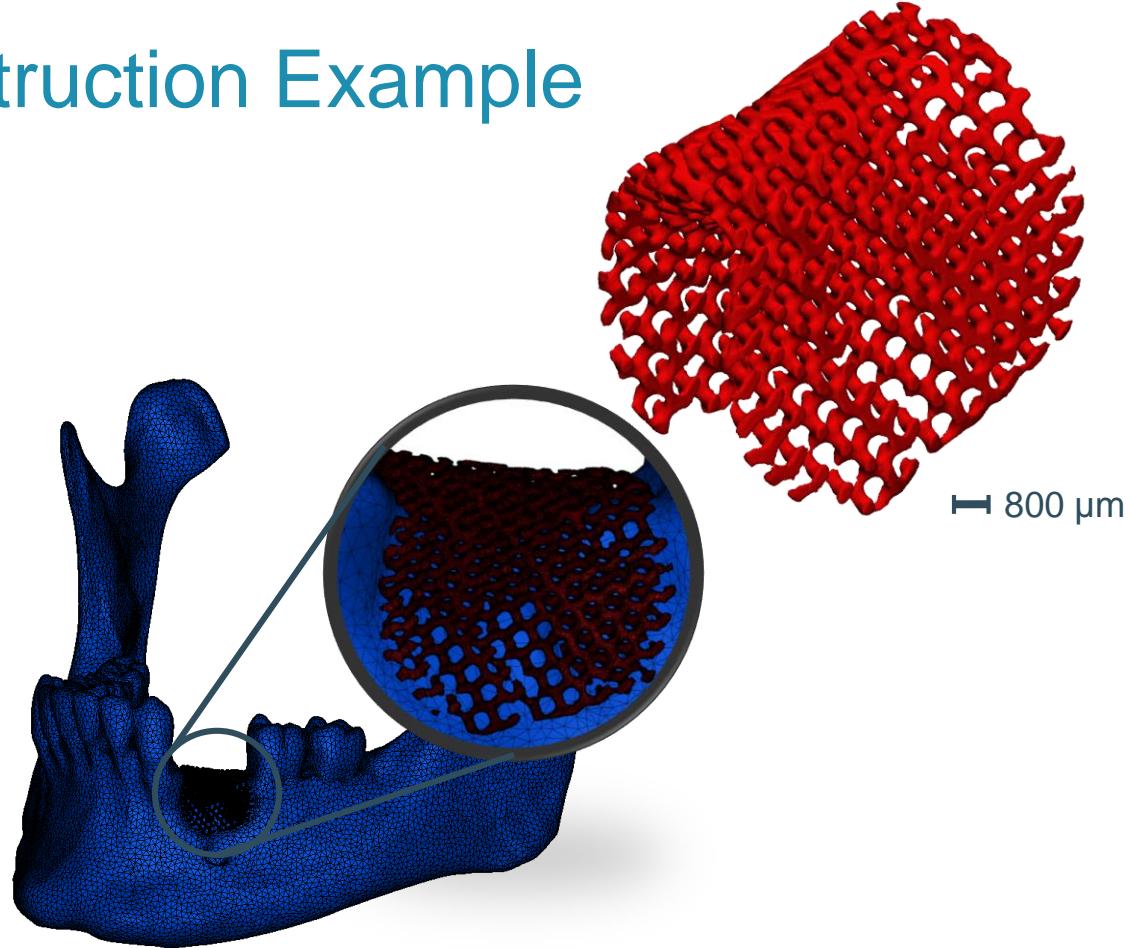
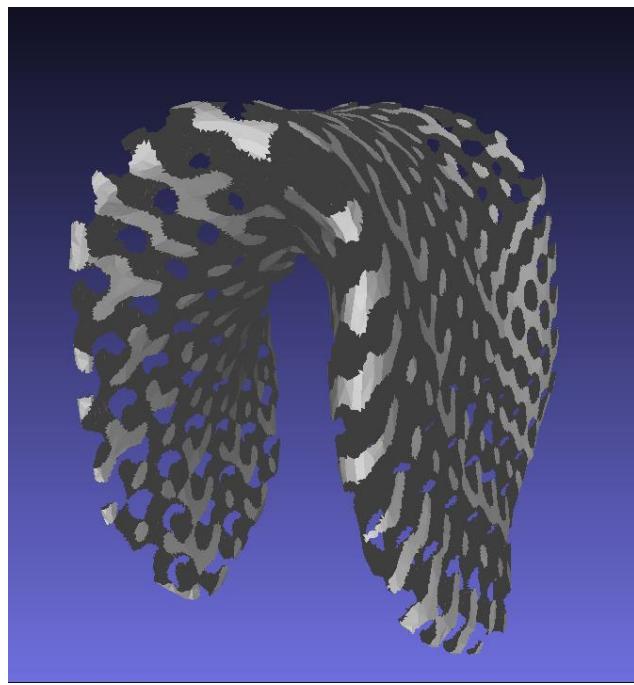
- Applying an implicit function and trimming mesh using Mmg
- Various shapes suitable for tissue engineering scaffolds



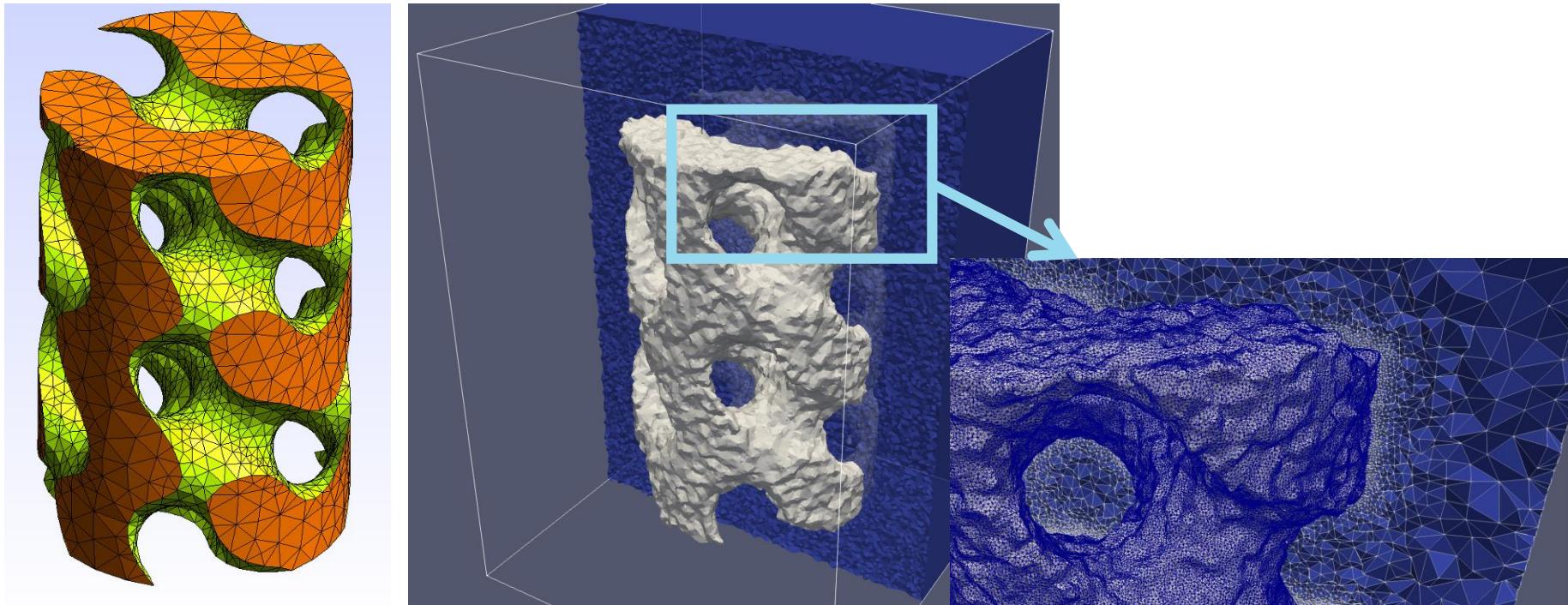
Acetabular Cup Example



Jaw Bone Reconstruction Example



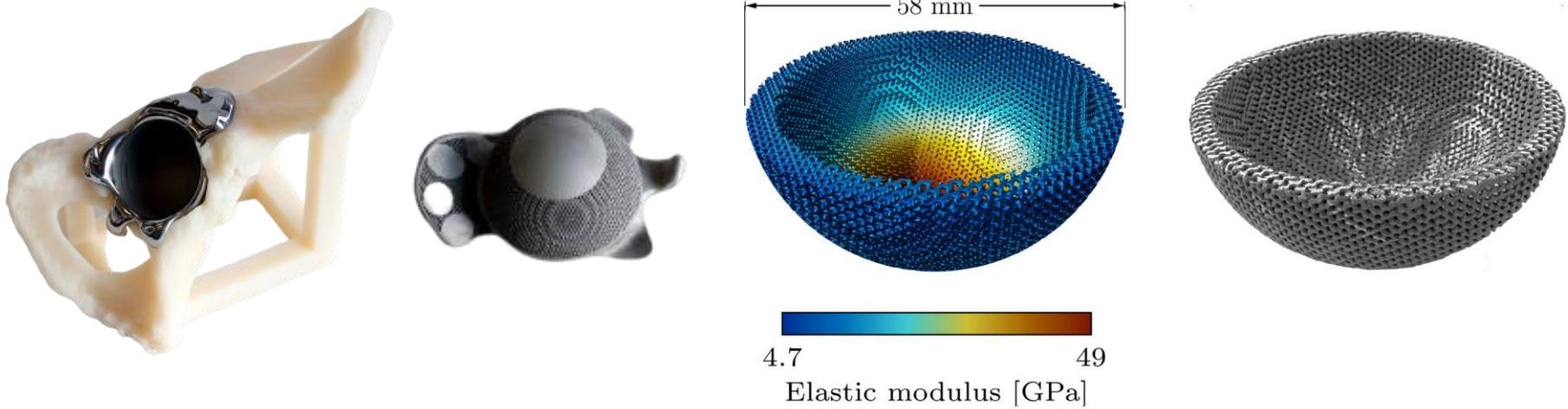
Embedding Mesh & Refinement



HPC case study: biodegradation simulation for a patient-specific implant

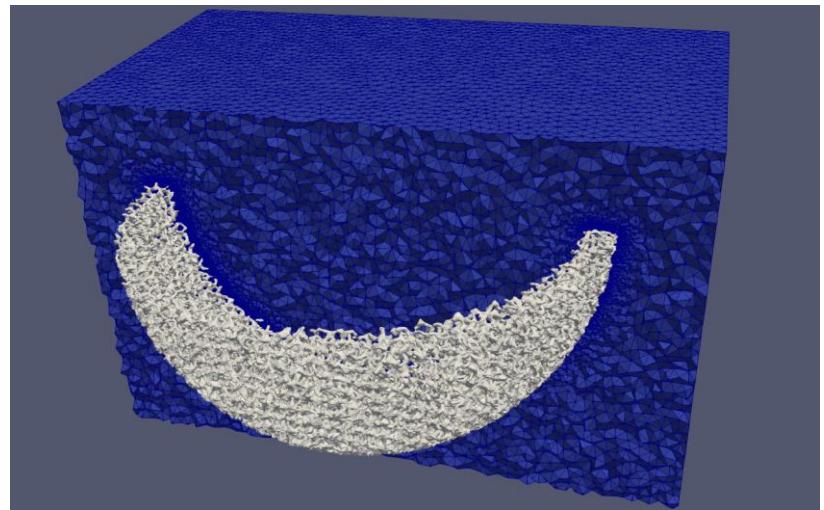
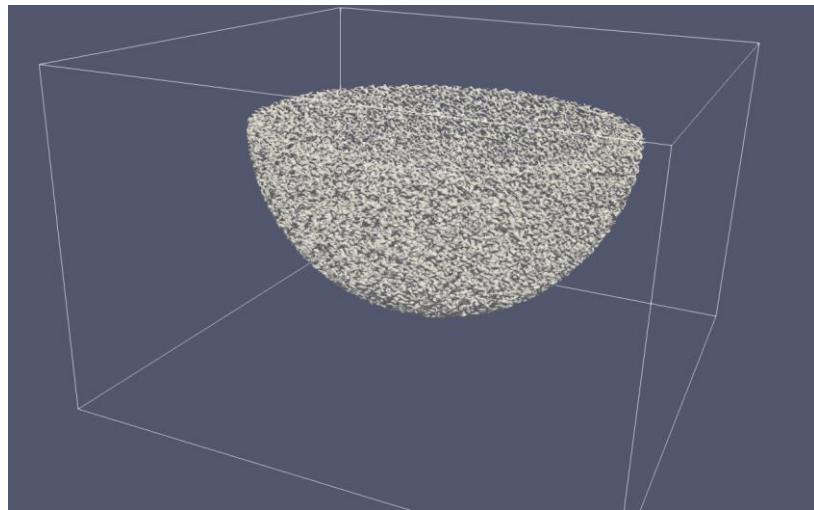
Porous Acetabular Cup

- The cup of hip implants, infilled with TPMS lattice structures to match a desired stiffness distribution



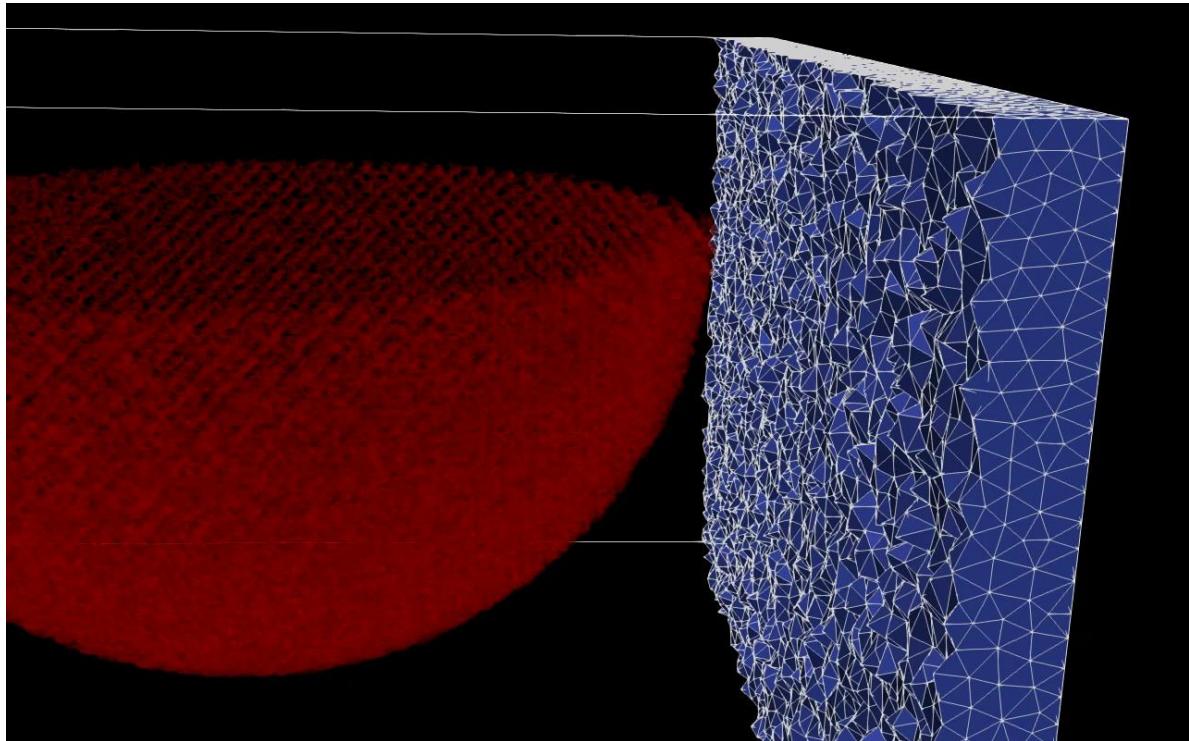
Simulation Setup

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



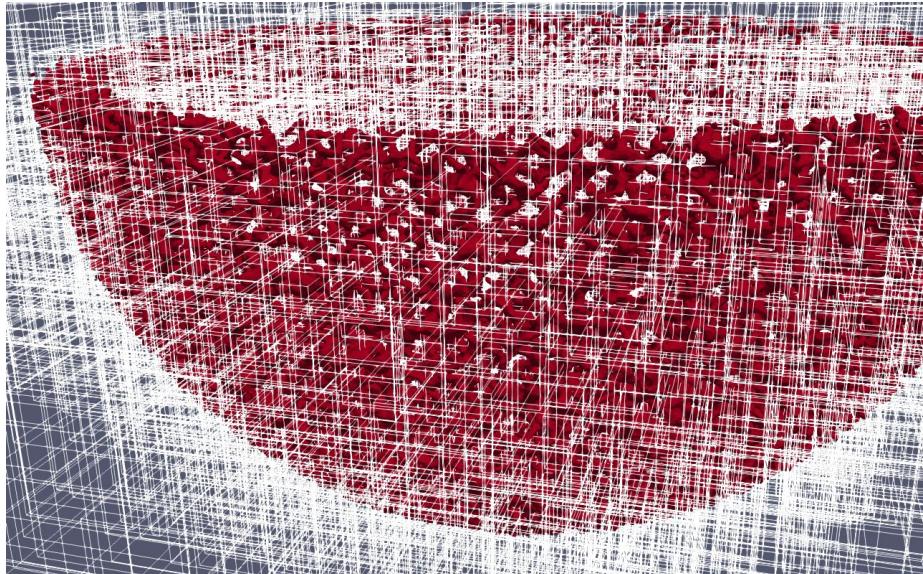
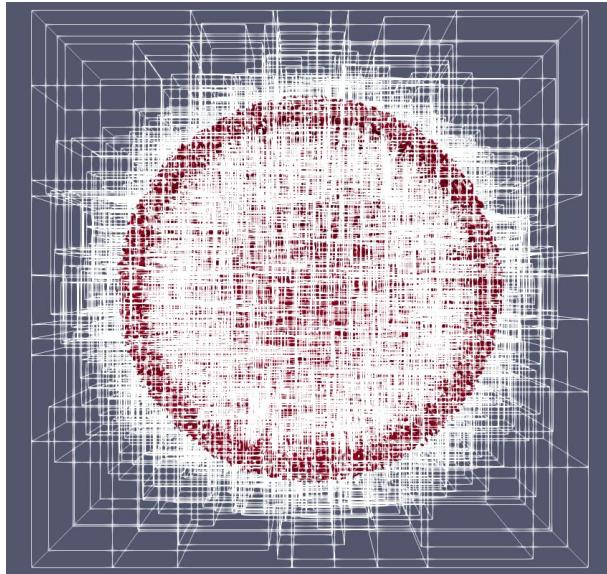
The Computational Mesh

- Containing ~45M elements



Mesh Decomposition for HPC

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

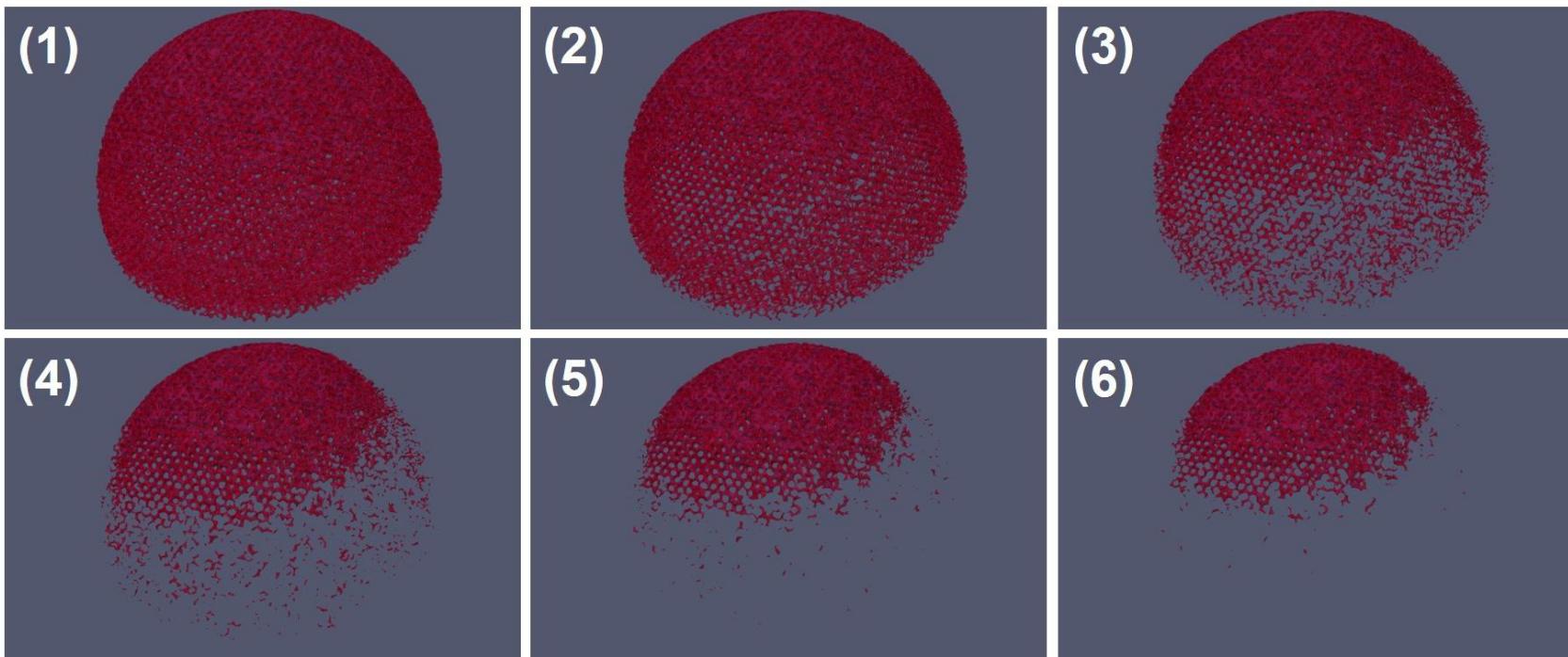


Degradation Behavior Result

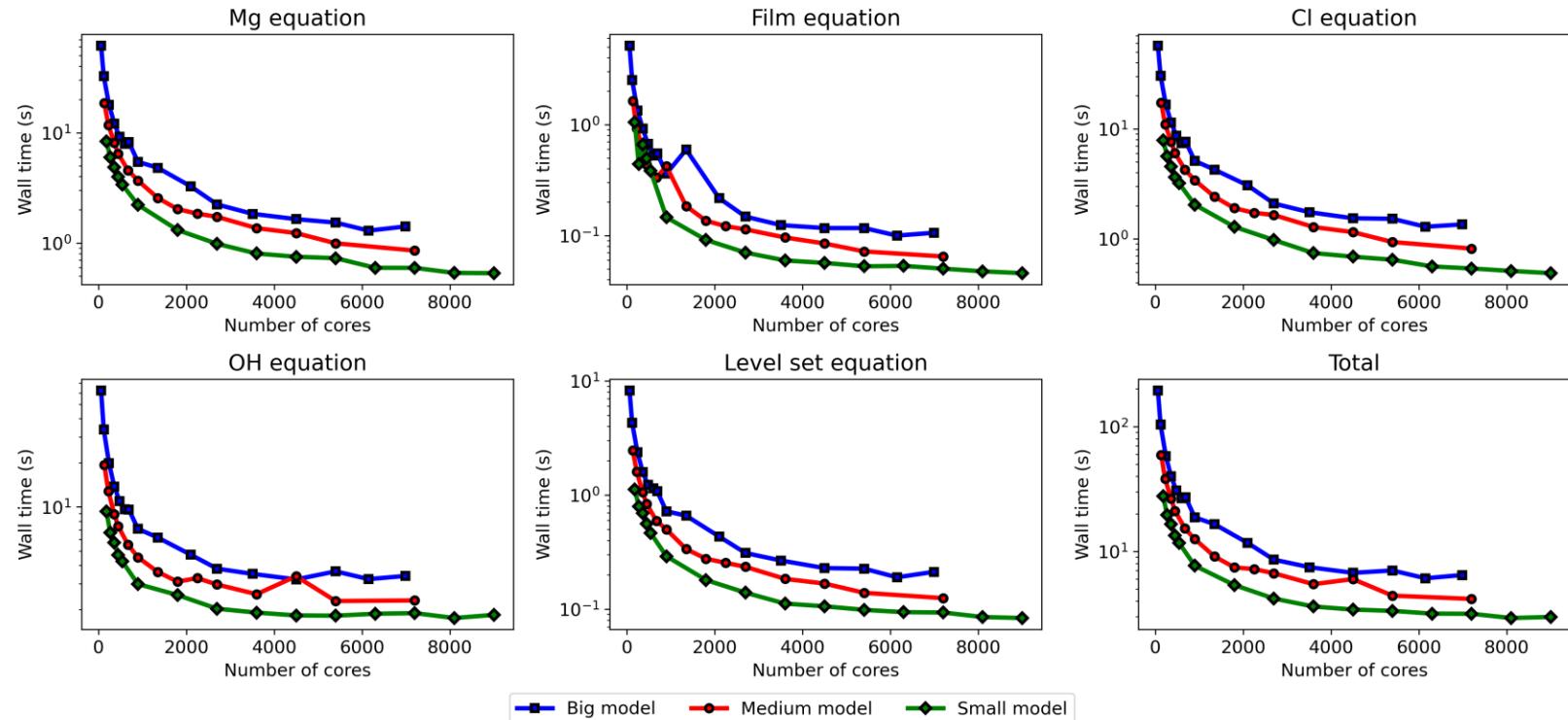
- Visualization done using 128 CPU cores



Degradation Behavior Result



Strong Scaling Tests



Open science and outreach

Outreach & Educational Content

- Details of employed techniques in simplified language
- Trainings on open source computational modeling



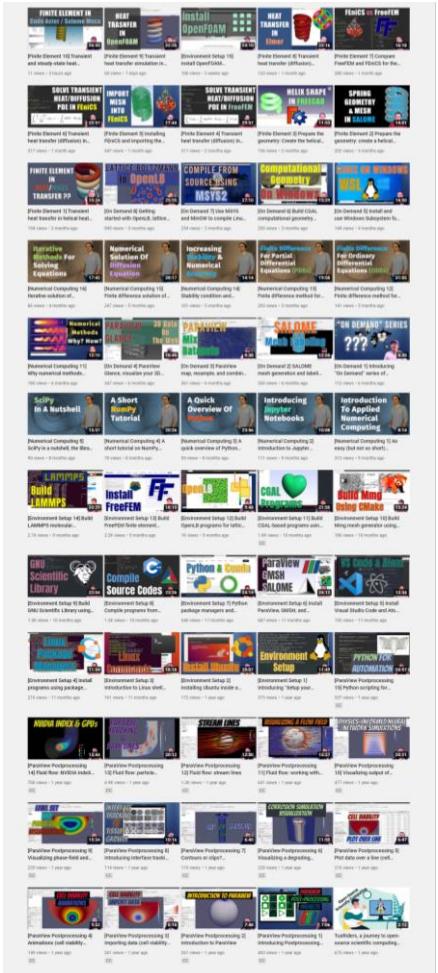
<http://TuxRiders.com>



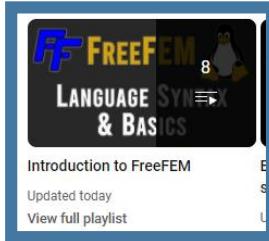
<https://youtube.com/TuxRiders>



TuxRiders



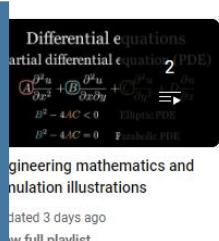
FreeFEM Series



Introduction to FreeFEM

Updated today

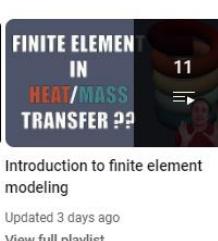
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1
LANGUAGE SYNTAX & BASICS 28:52

[FreeFEM 1] Introduction to FreeFEM: language syntax and environment

TuxRiders • 470 views • 1 month ago



2
2D MESH GENERATION 23:28

[FreeFEM 2] 2D mesh generation in FreeFEM

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3
3D MESH GENERATION 24:00

[FreeFEM 3] 3D mesh generation and handling in FreeFEM

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4
FINITE ELEMENT SPACES 22:41

[FreeFEM 4] Finite element spaces and function approximation in FreeFEM

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5
WEAK FORMULATION & SOLVING PDE 21:14

[FreeFEM 5] Implementing weak formulation to solve partial differential equations in FreeFEM

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6
ADAPTIVE MESH GENERATION 20:41

[FreeFEM 6] Adaptive mesh generation in FreeFEM

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7
VISUALIZATION & I/O 18:06

[FreeFEM 7] Visualization and input/output (IO) operations in FreeFEM

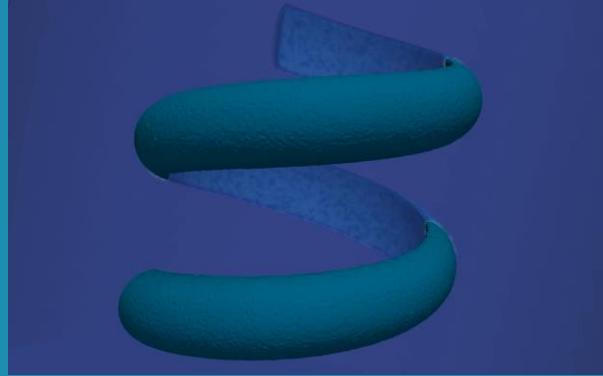
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8
REGIONS & SUB-DOMAIN 22:36

[FreeFEM 8] Regions and sub-domains to define variable material properties and initial conditions

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Thank you for your attention



<https://mbarzegary.github.io>



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