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

Mojtaba Barzegari, Laura Lafuente-Gracia, Liesbet Geris

Biomechanics Section, Department of Mechanical Engineering,

KU Leuven, Leuven, Belgium

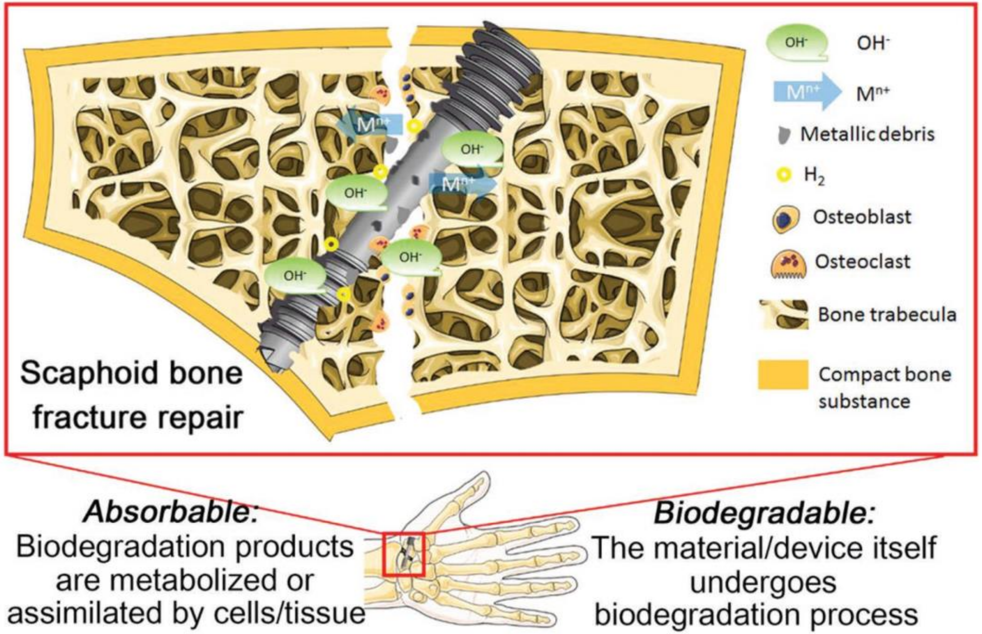
FreeFEM in Biomedical Engineering

- 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

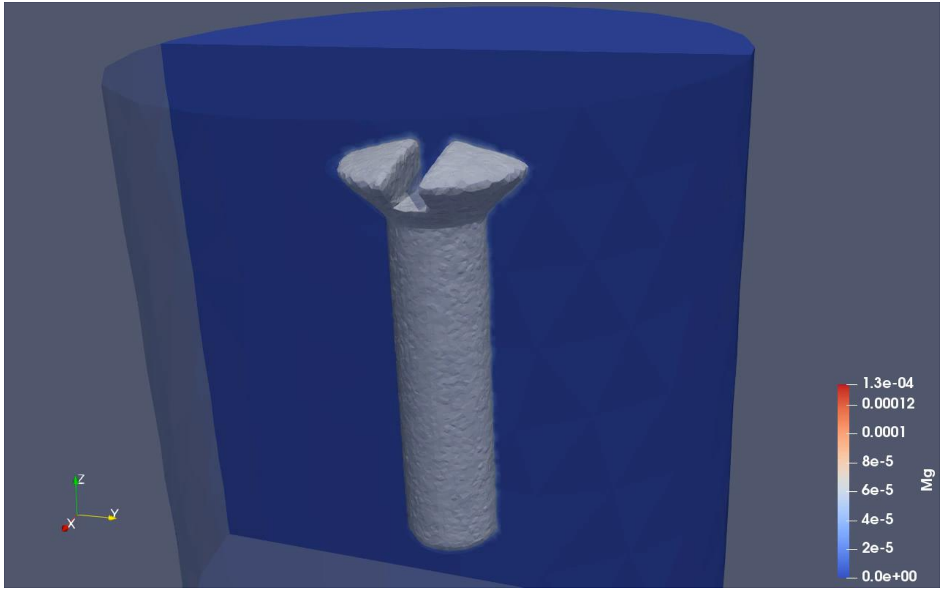
Biodegradable Metals

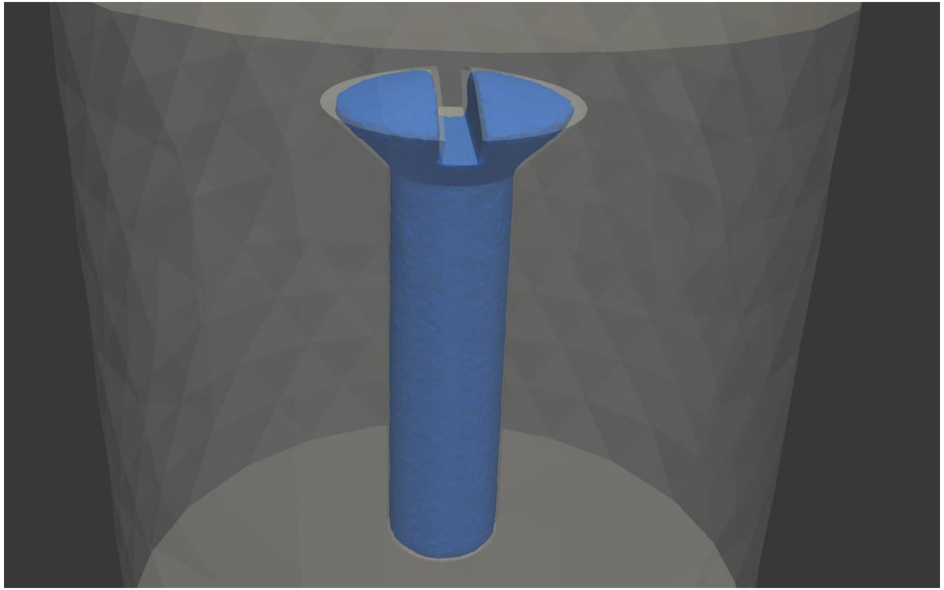
- Dissolve upon fulfilling the mission to assist tissue healing
- The degradation behavior should be tuned/optimized
- A set of reaction-diffusion-advection PDEs describing the chemistry of biodegradation
- Level-set for tracking the moving corrosion front



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

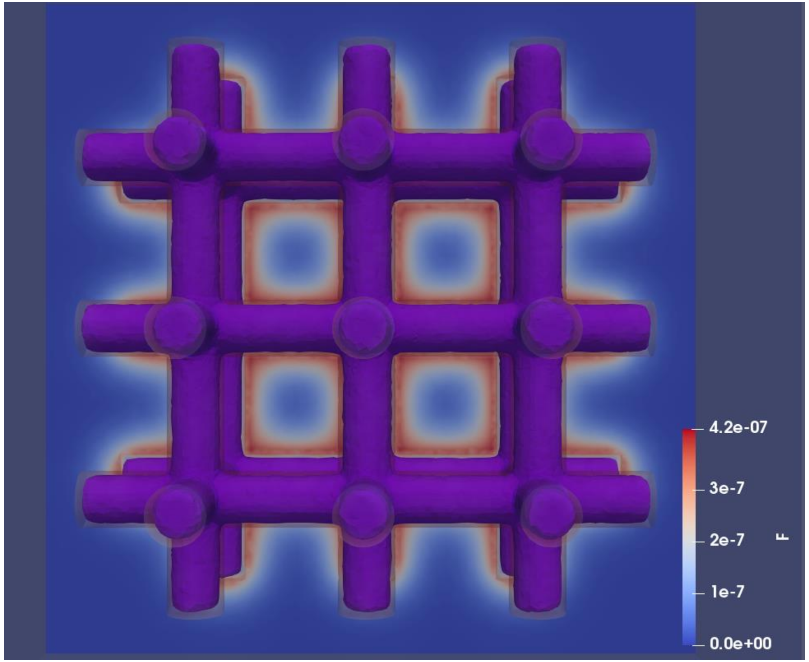
Orthopedics Screw Degradation

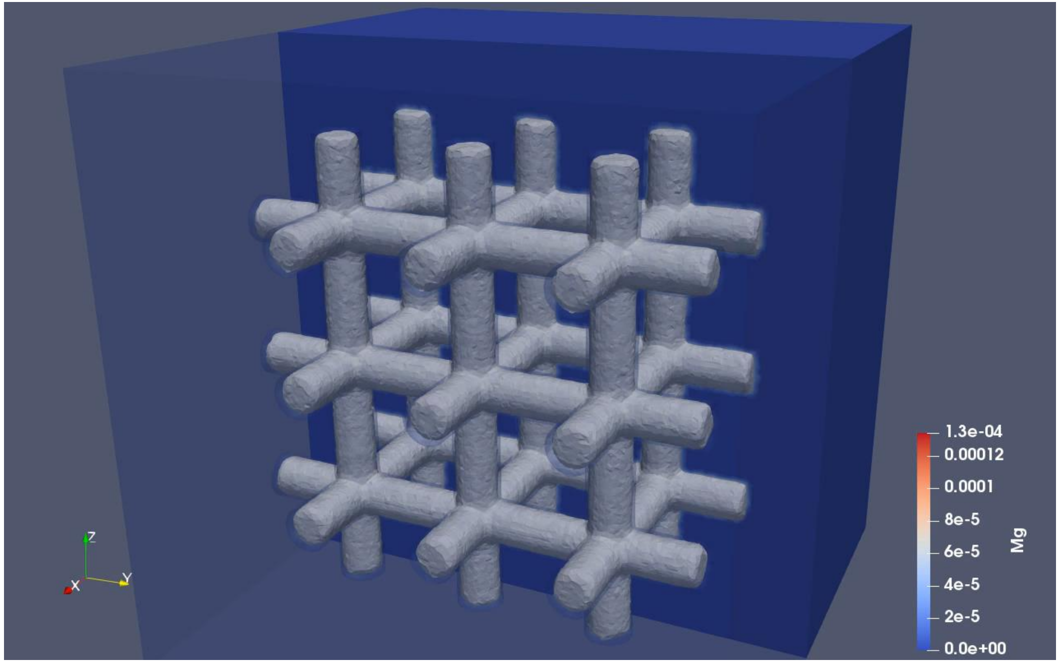




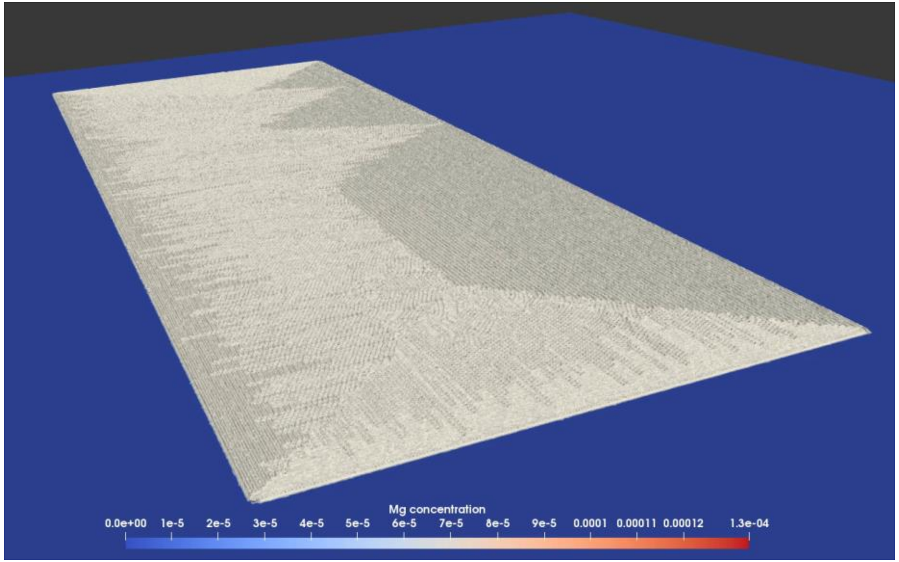
KU LEUVEN

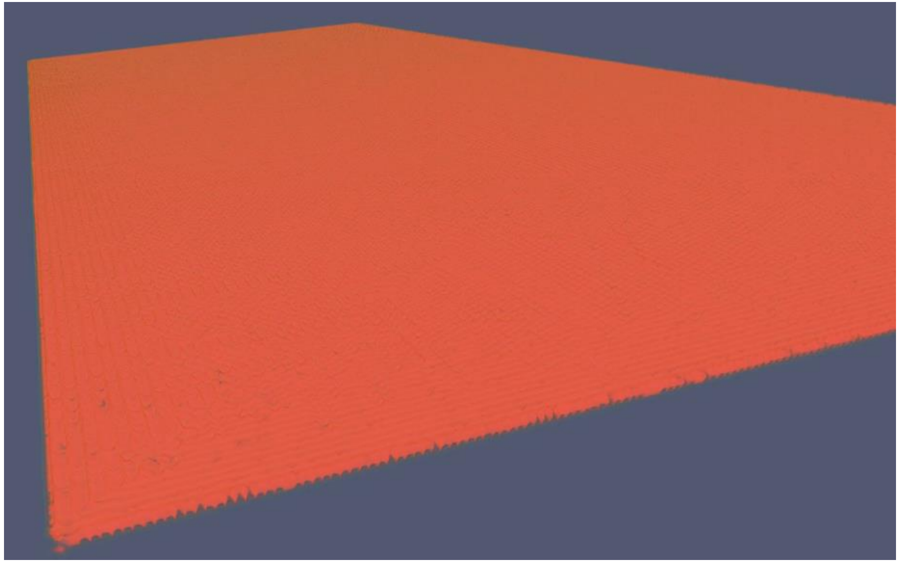
Porous Scaffold Degradation





Narrow Cuboid

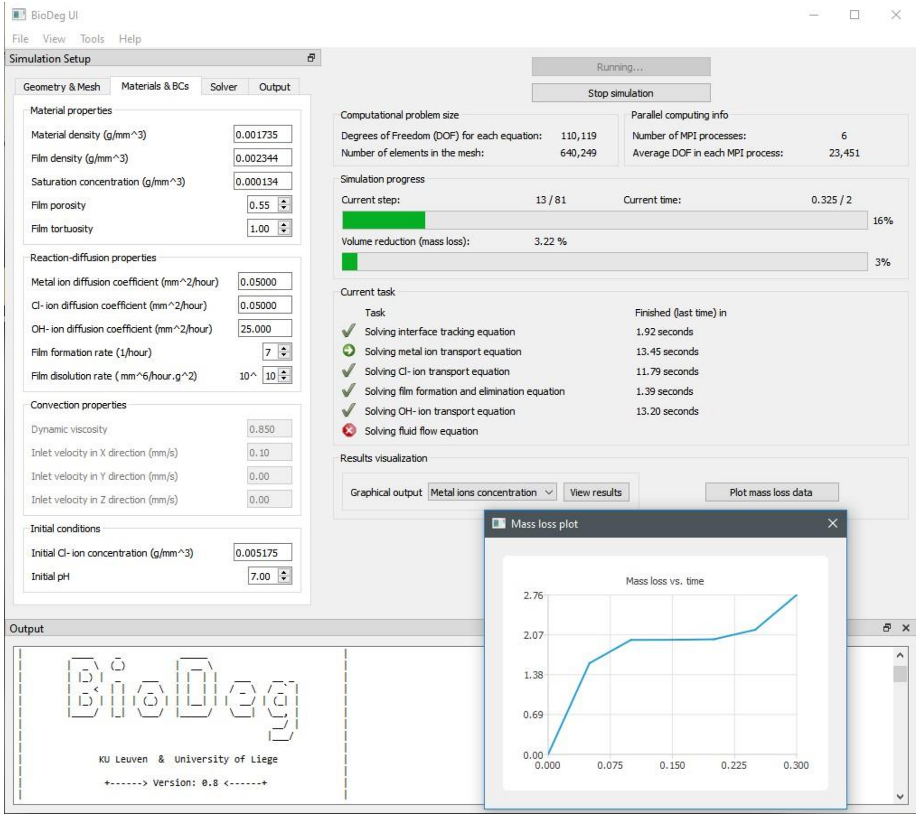




(Barzegari et al., Corrosion Science, 190, 2021)

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

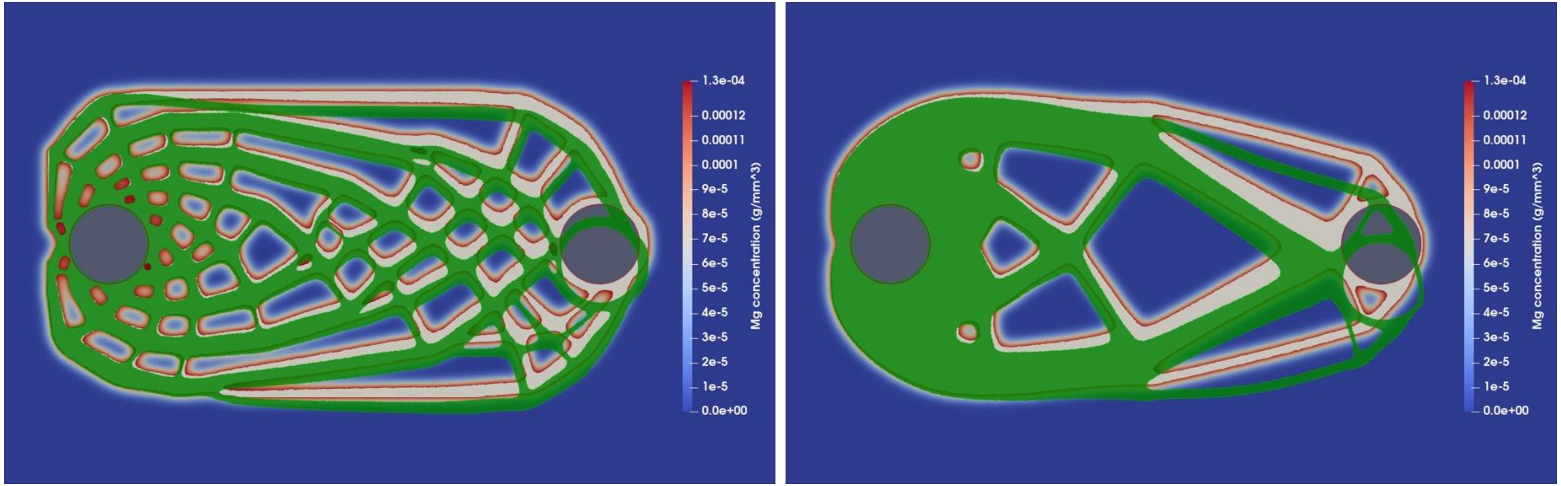


https://github.com/mbarzegary/BioDeg-UI

KU LEUVEN

Model Integration

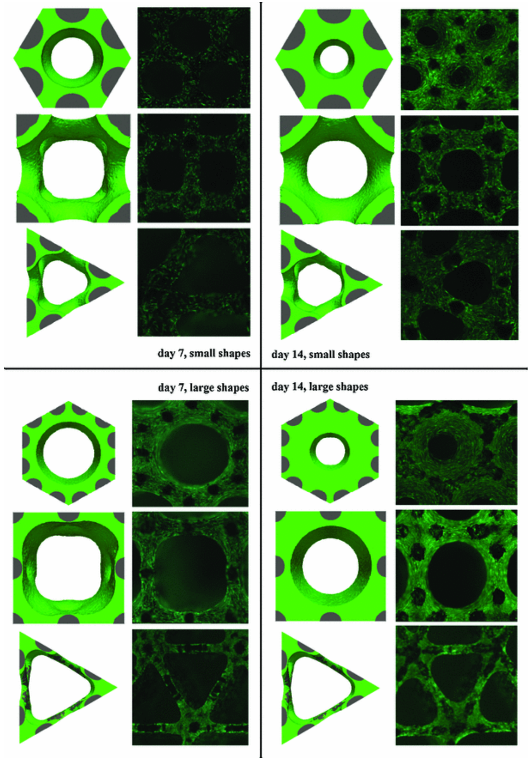
- Coupled models of topology optimization and metals corrosion for optimizing the shape of biodegradable infilled structures



Computational modeling of tissue regeneration and growth

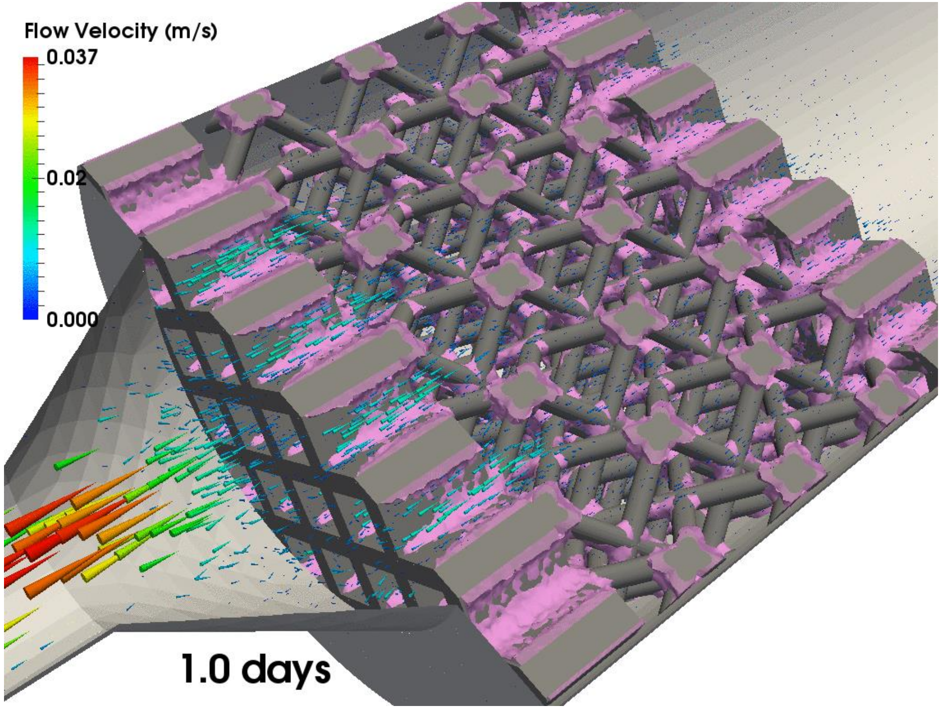
Curvature-based Tissue Growth

- 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

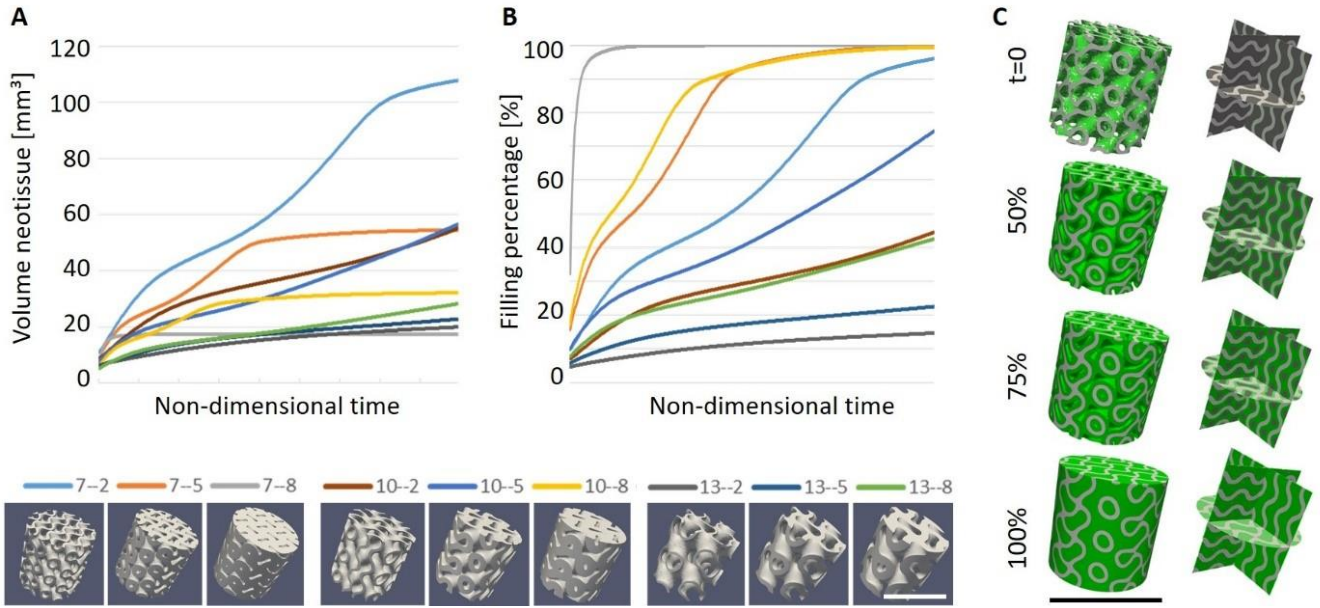


(Guyot et al., Biomech Model Mechanobiol., 13, 2014)

Tissue Regeneration in Bioreactors

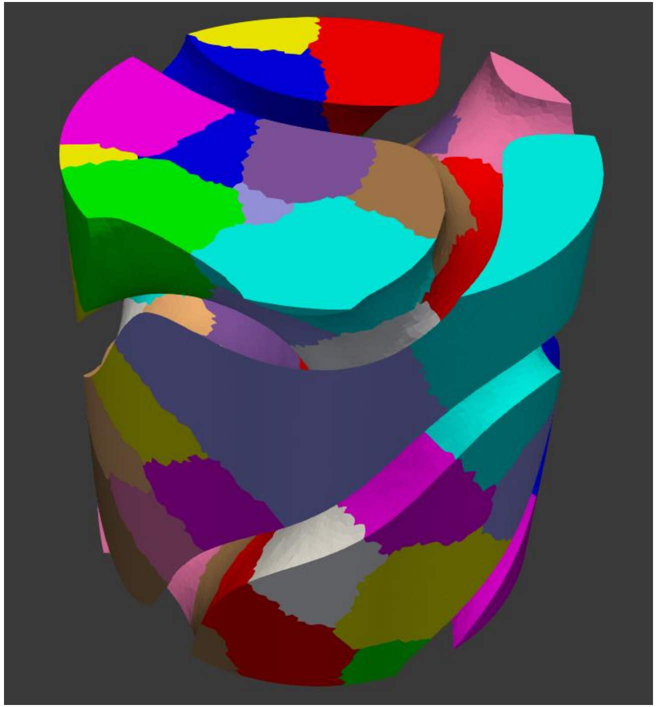


Tissue Growth on Various Scaffolds



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

Parallel Implementation of Interface Tracking

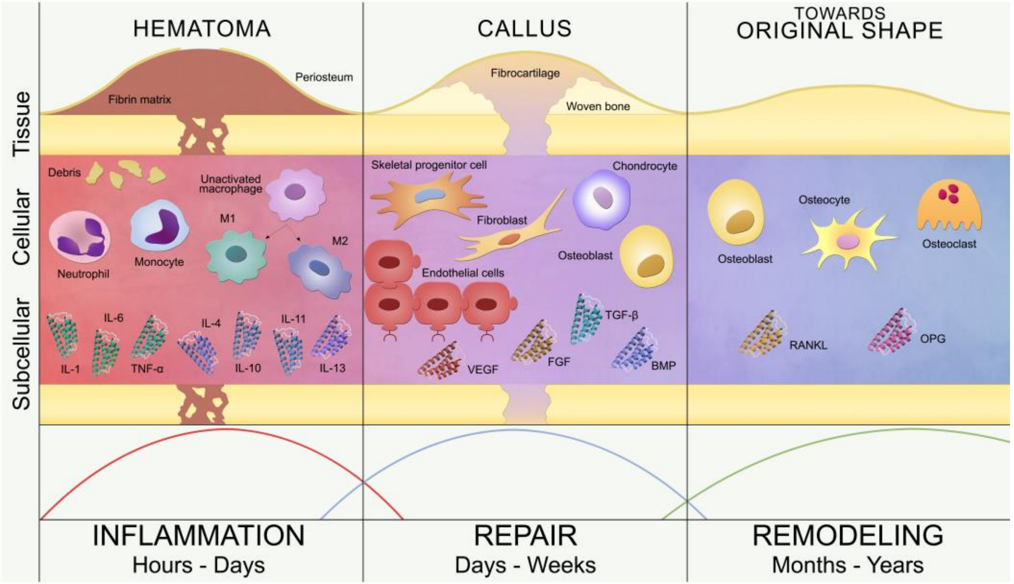


KU LEUVEN

Computational modeling of bone fracture healing

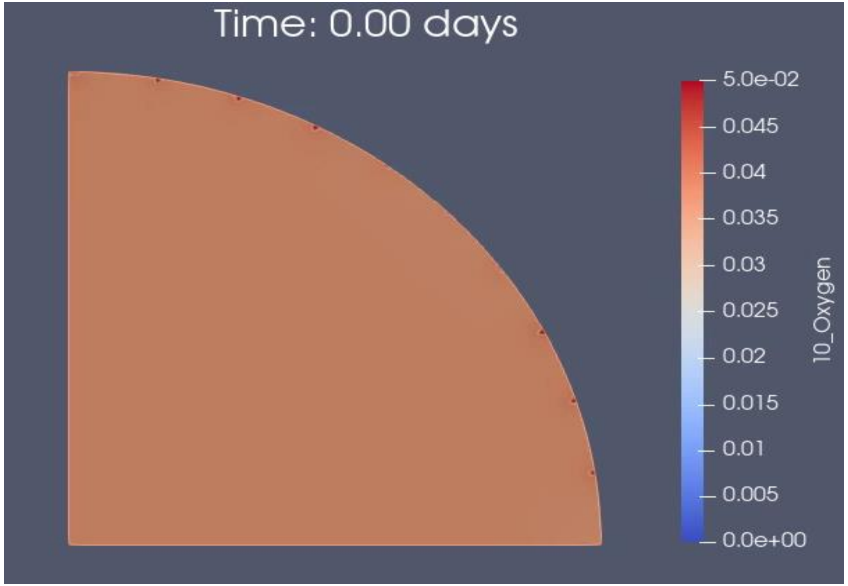
Repair Phase of Healing Process

- 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

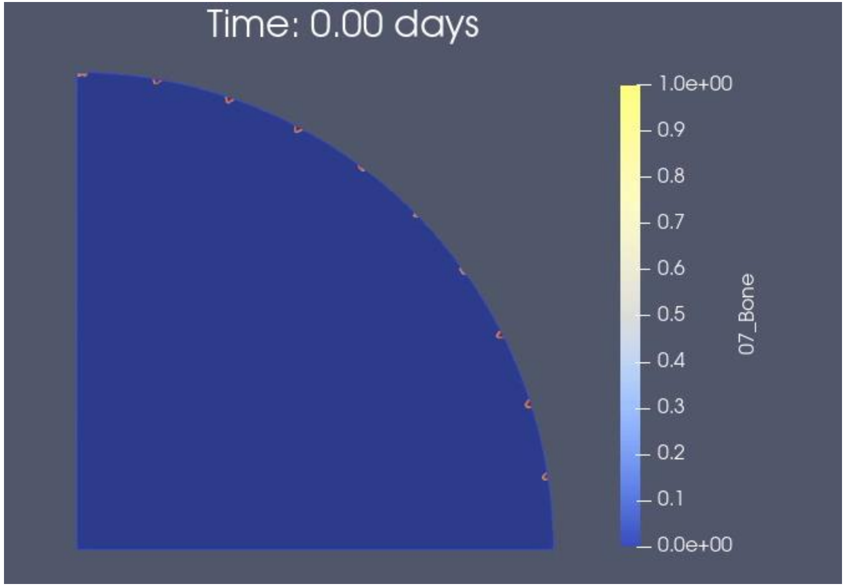


(Lafuente-Gracia et al., Front. Bioeng. Biotechnol, 2021)

Bone Regeneration for Mandibular Defects

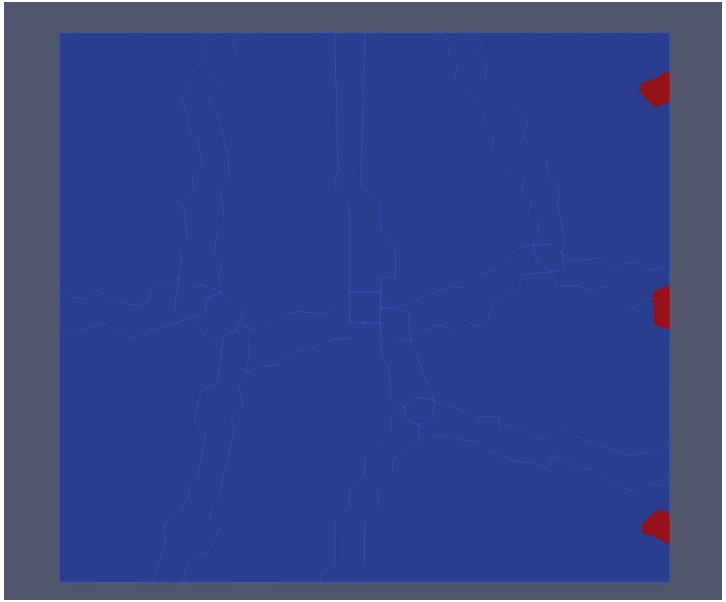


Vascular network & oxygen supply

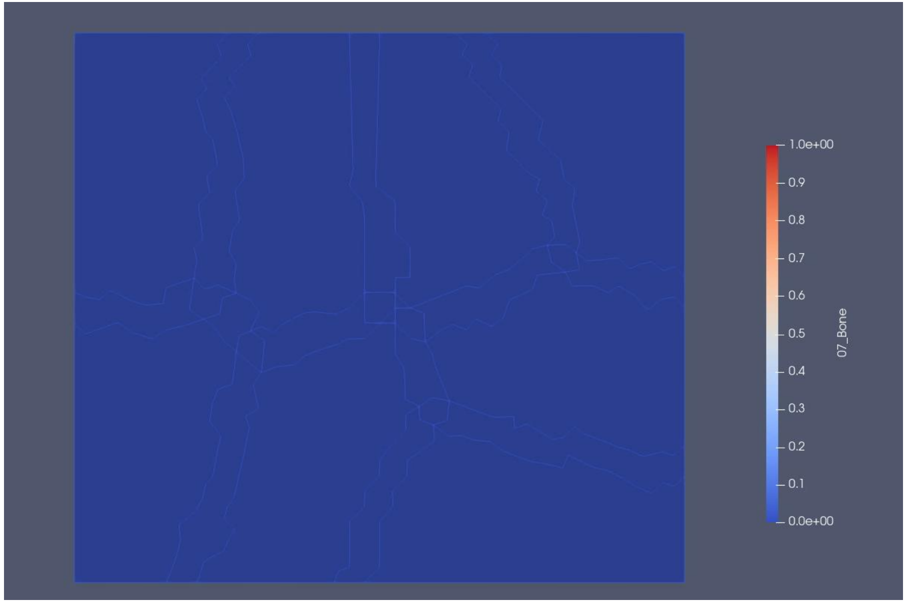


Bone formation

Parallelized Coupled FE-CA Model



Vessels growth

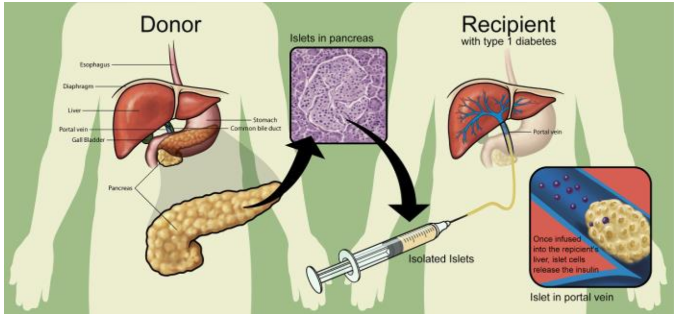


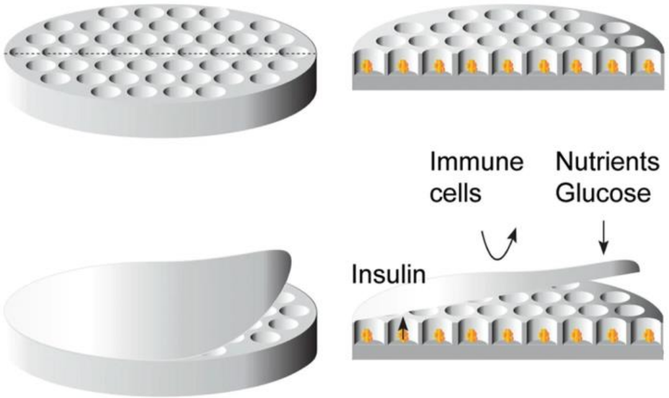
Bone formation

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

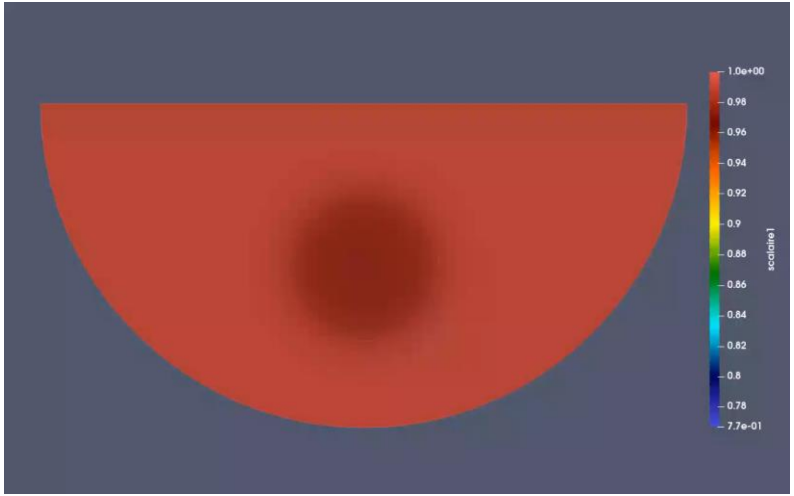


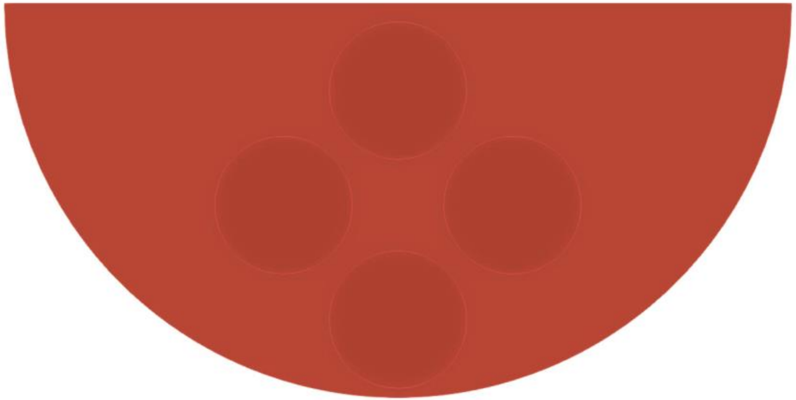


(sources: M.A. Naftanel et al., 2004, and K. Skrzypek et al., 2017)

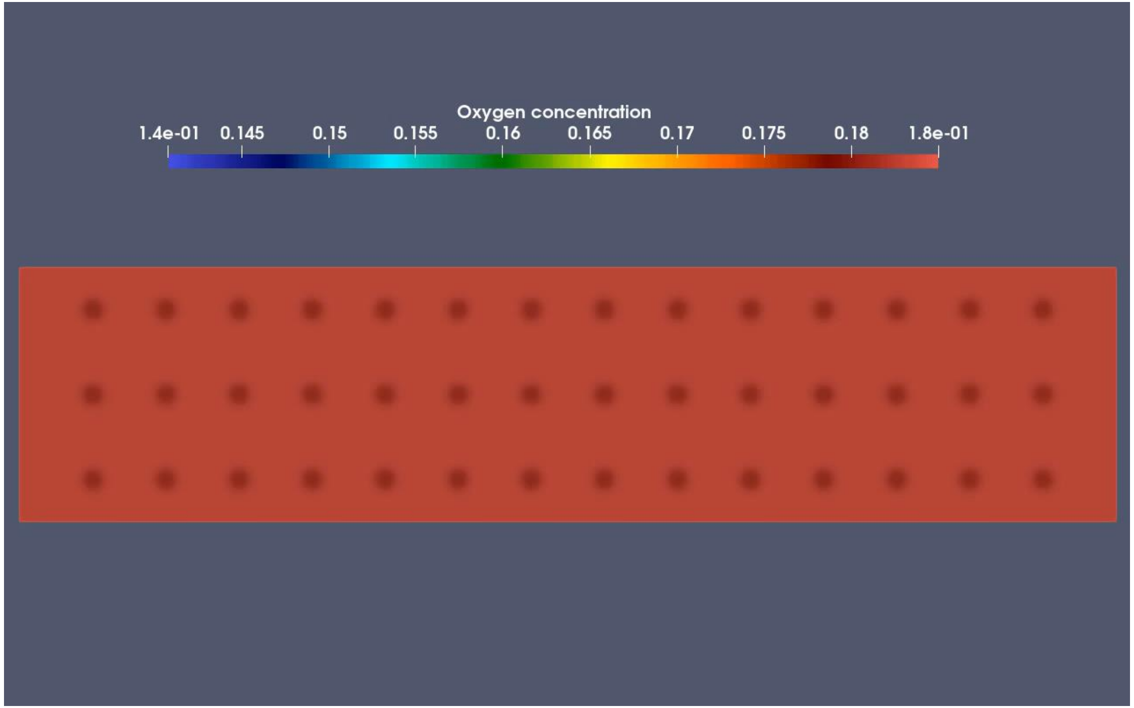
KU LEUVEN

Single Micro-device Simulations





Islets Group, Multiple Wells

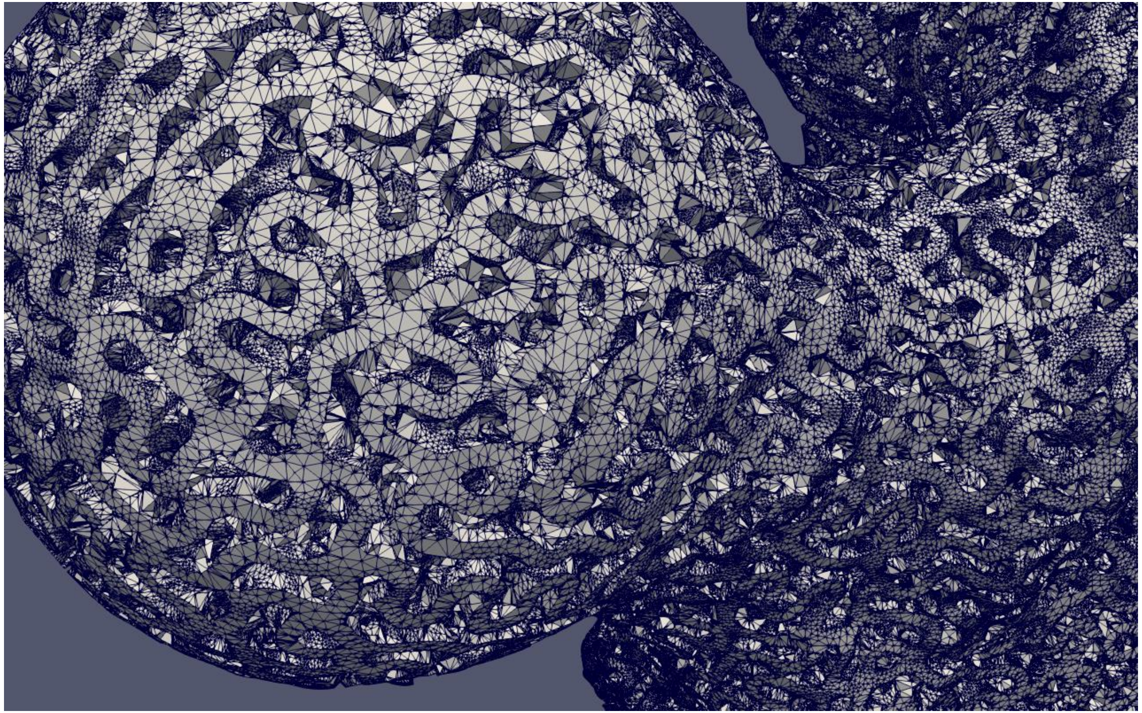


KU LEUVEN

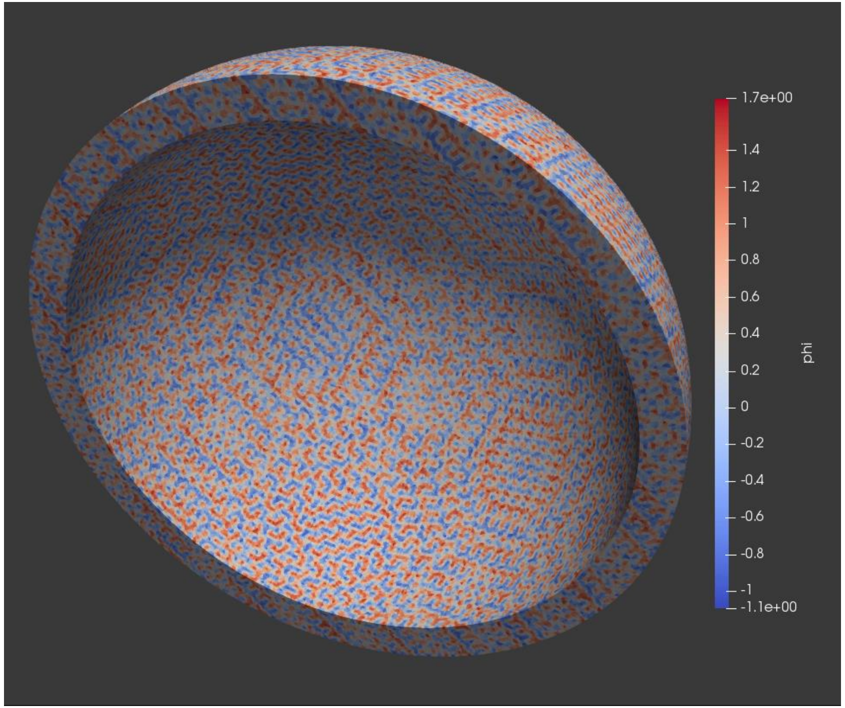
Geometry construction and mesh generation

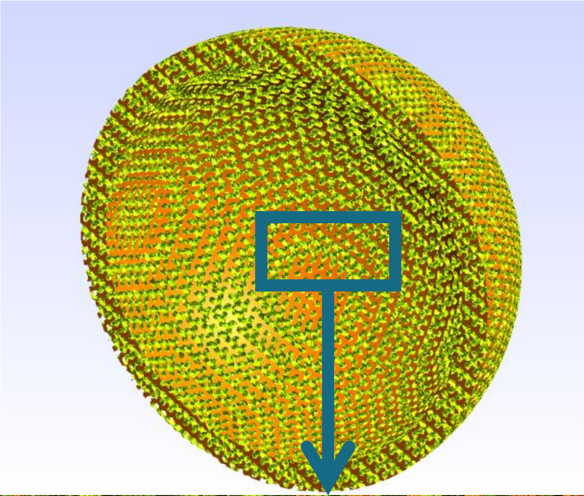
Implicit Mesh Constructions

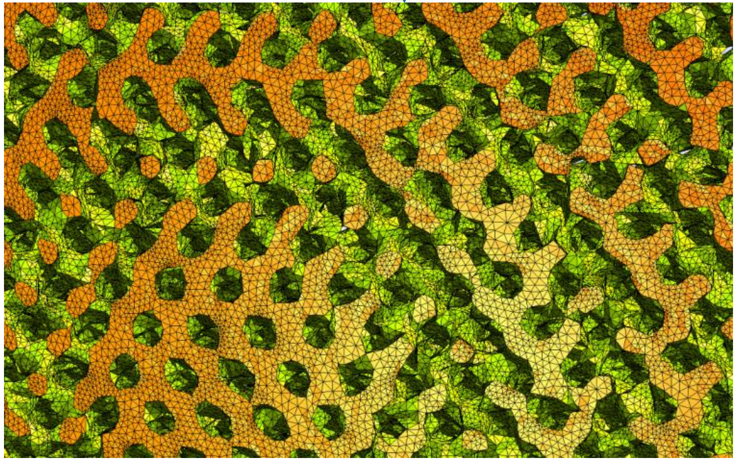
- Applying an implicit function and trimming mesh using Mmg
- Various shapes suitable for tissue engineering scaffolds



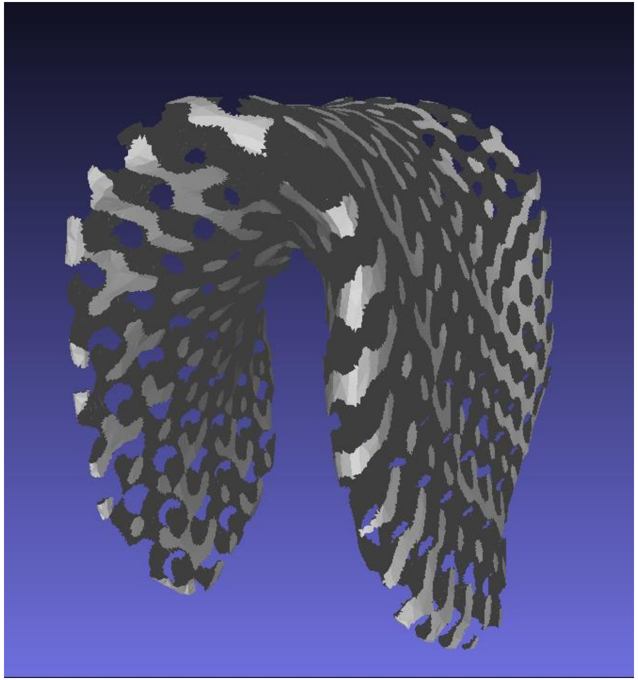
Acetabular Cup Example

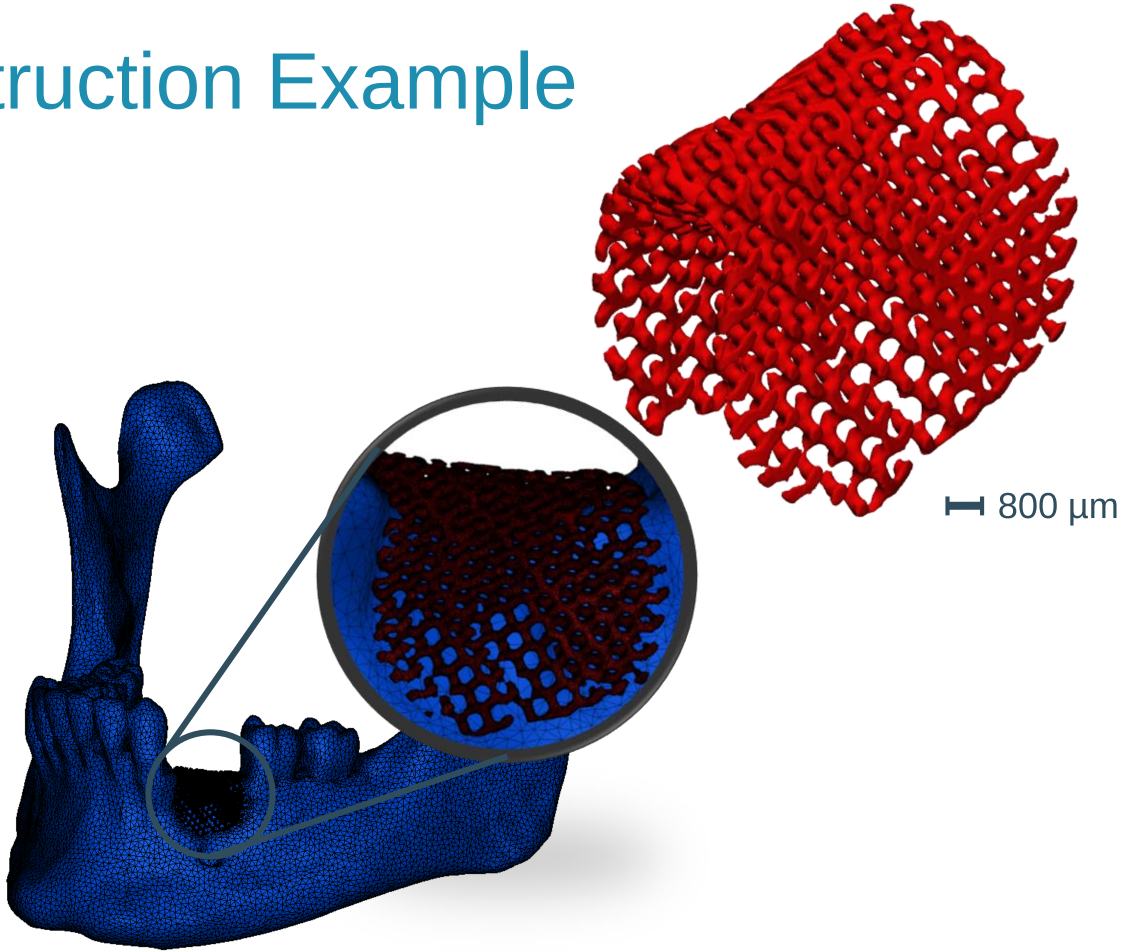






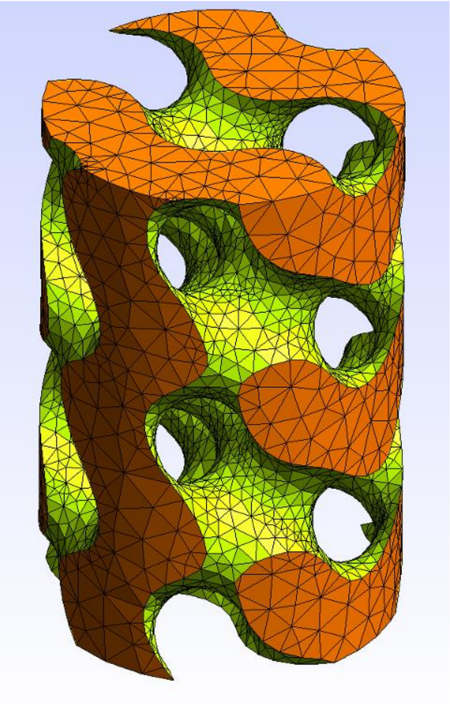
Jaw Bone Reconstruction Example

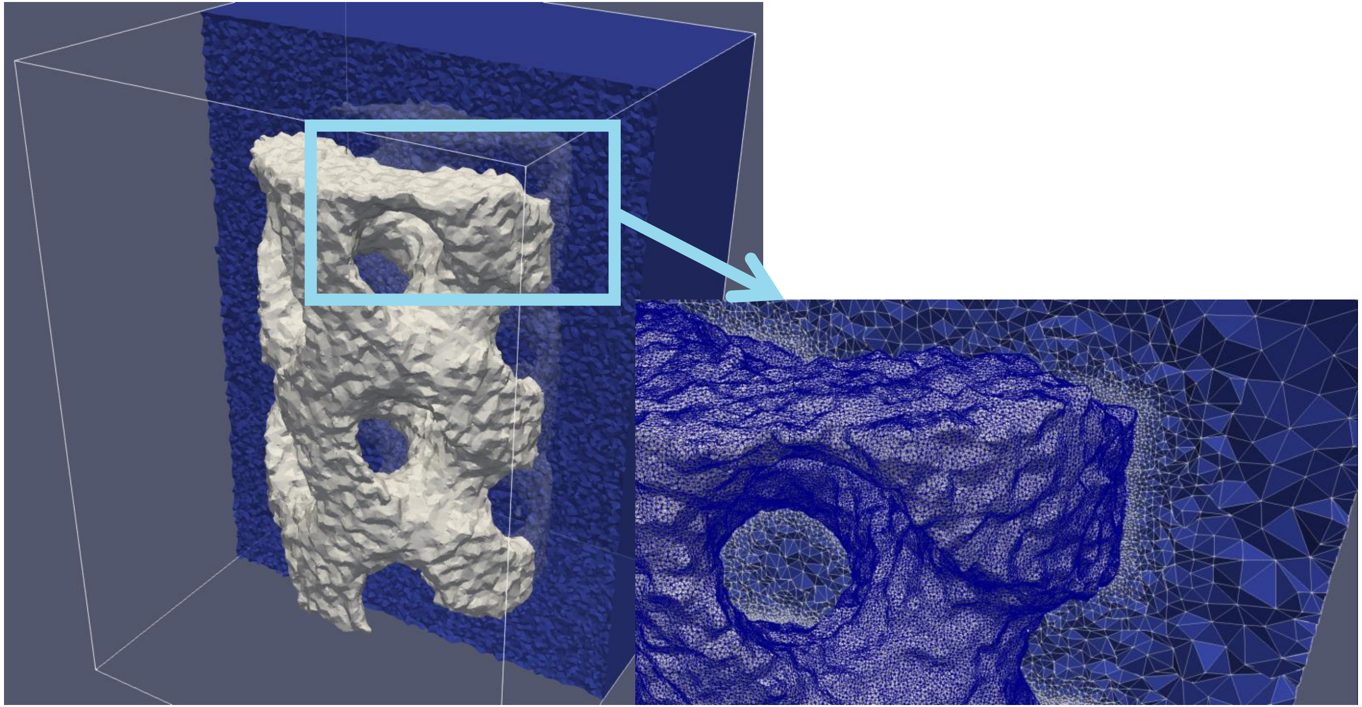




KU LEUVEN

Embedding Mesh & Refinement



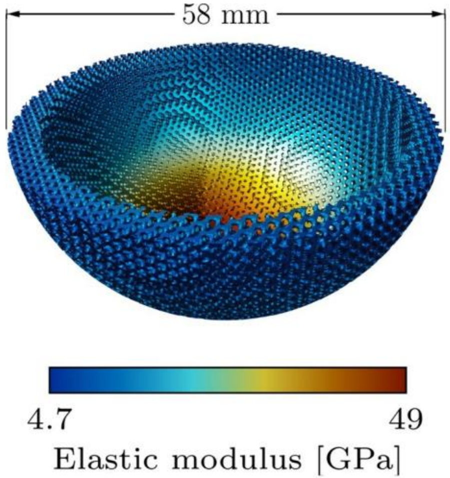


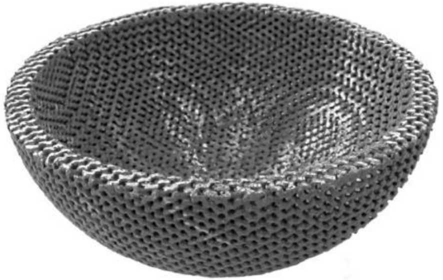
KU LEUVEN

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

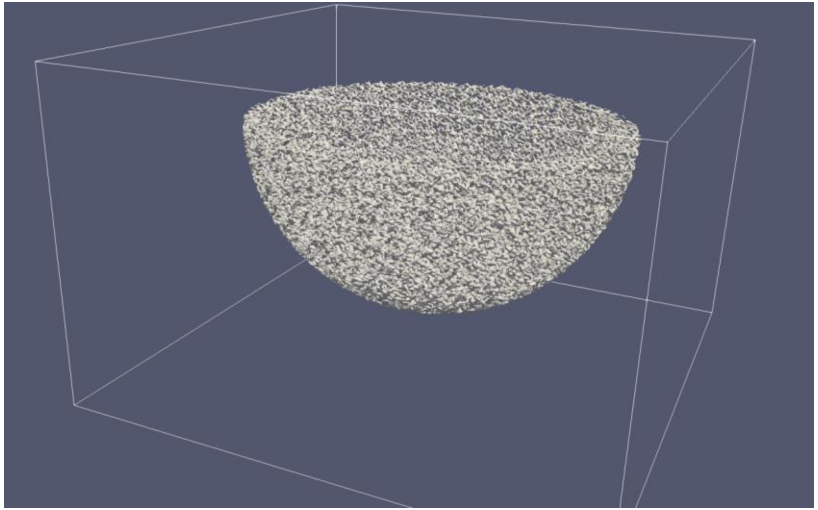


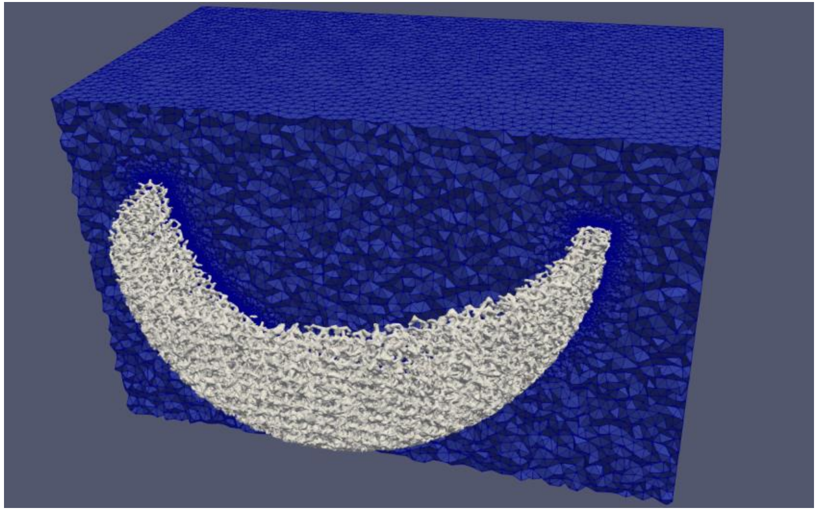


KU LEUVEN

Simulation Setup

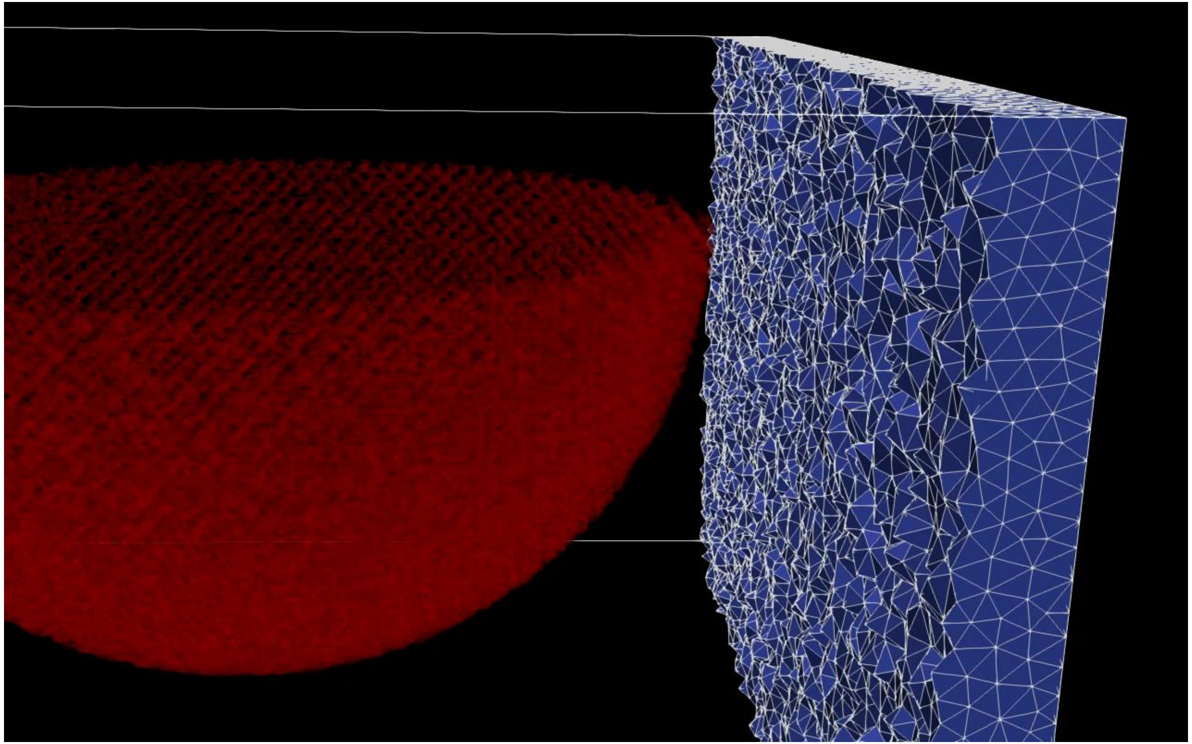
- Embedding the cup in a container and refine the mesh on its surface





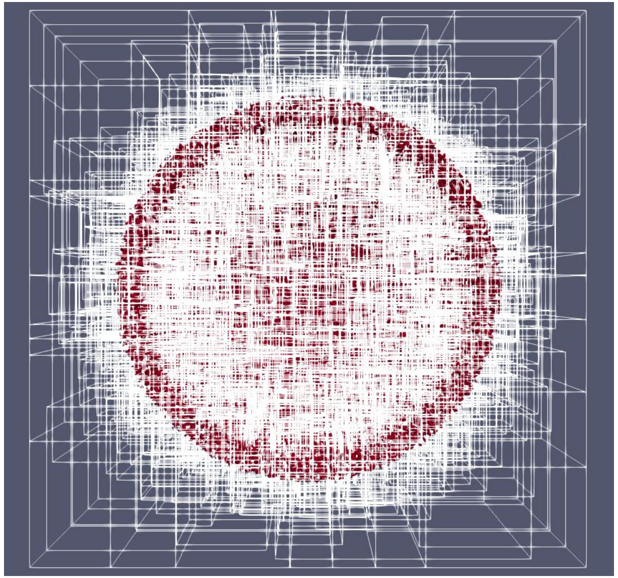
The Computational Mesh

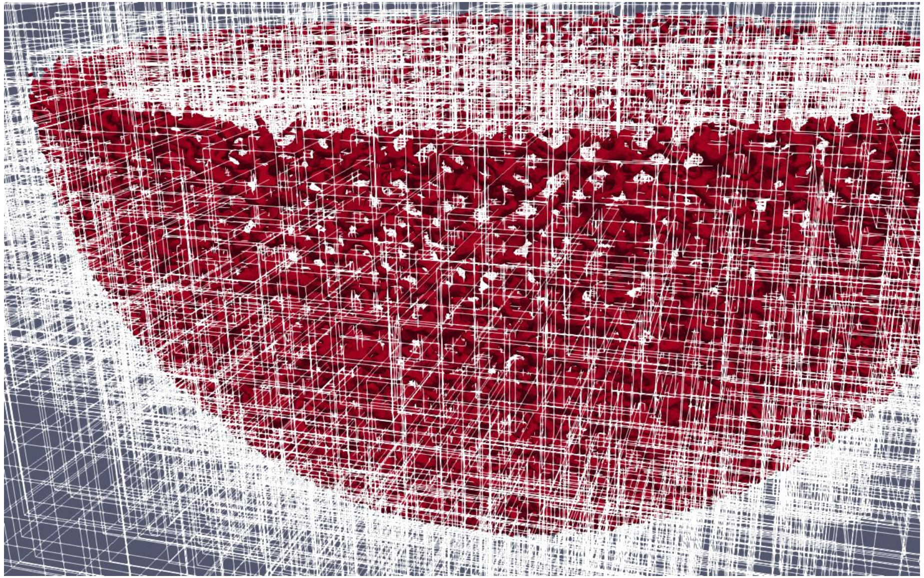
- Containing ~45M elements



Mesh Decomposition for HPC

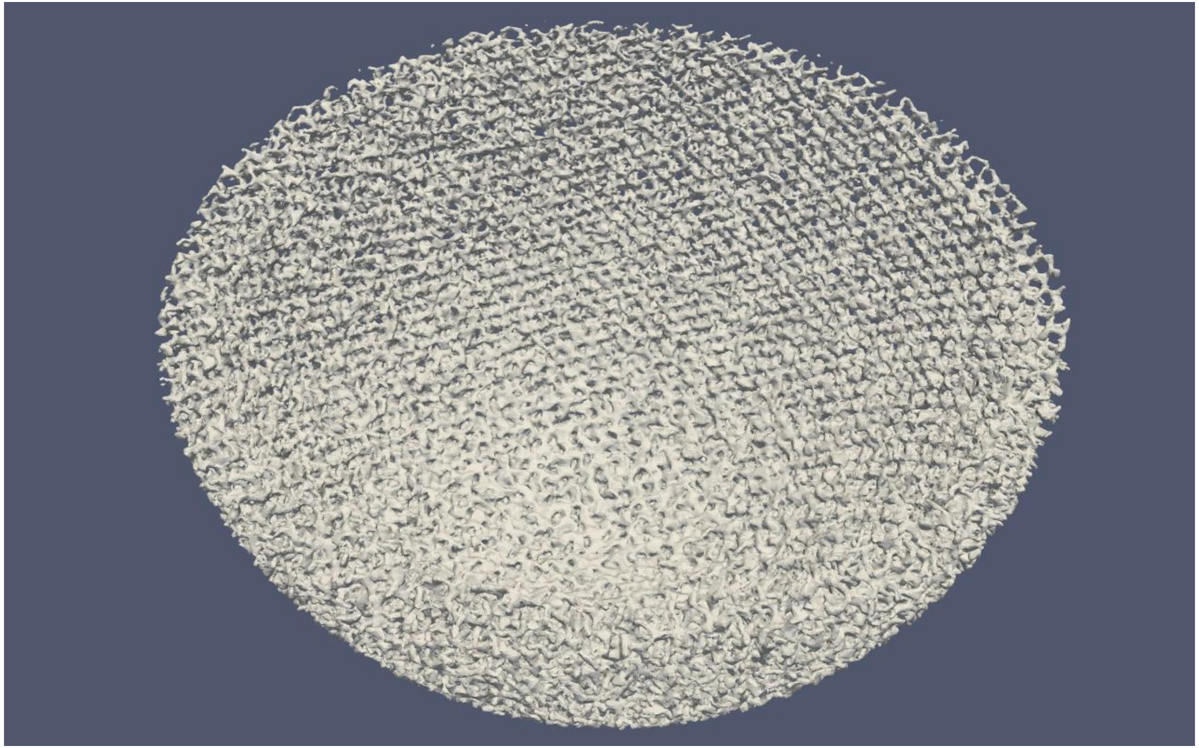
- Partitioning the mesh to be distributed to 2K - 8K CPU cores



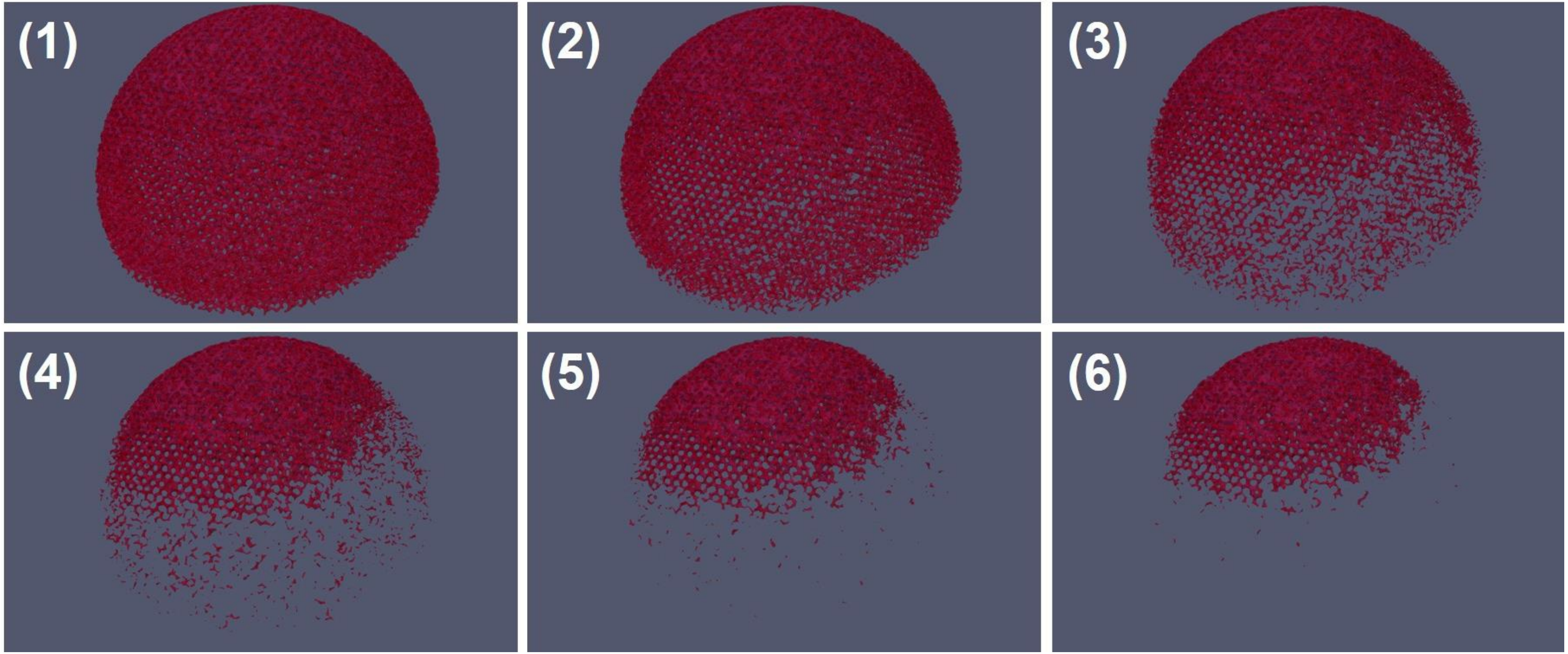


Degradation Behavior Result

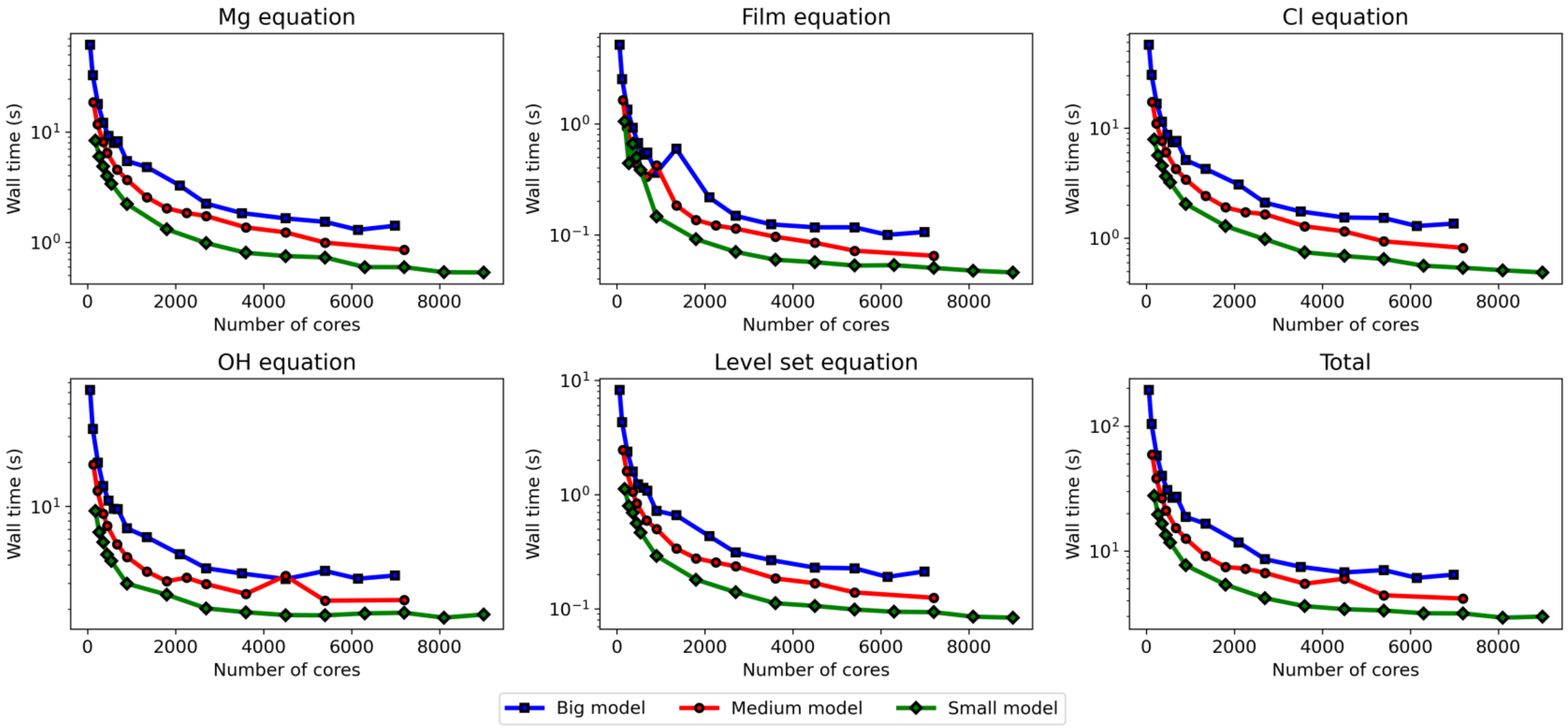
- Visualization done using 128 CPU cores



Degradation Behavior Result



Strong Scaling Tests



KU LEUVEN

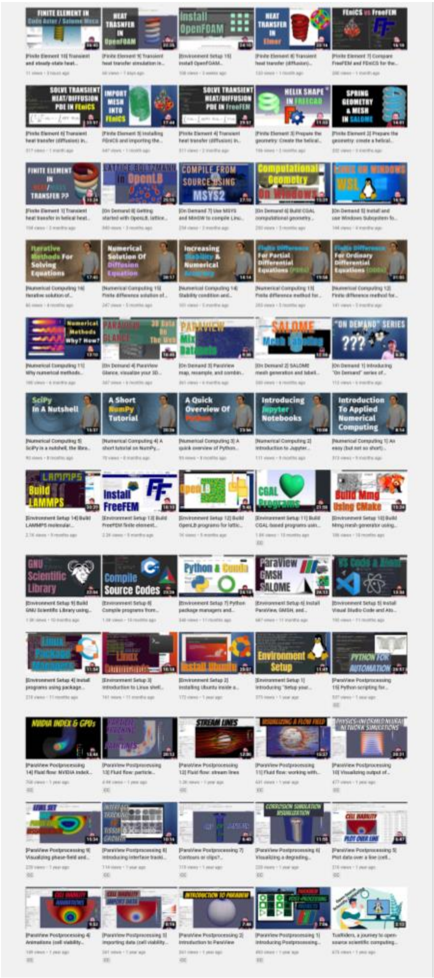
Open science and outreach

Outreach & Educational Content

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

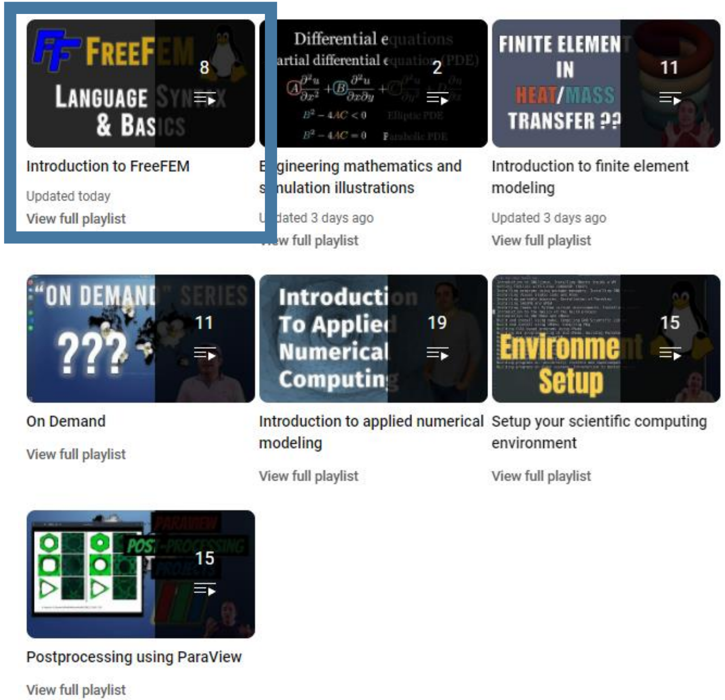
http://TuxRiders.com

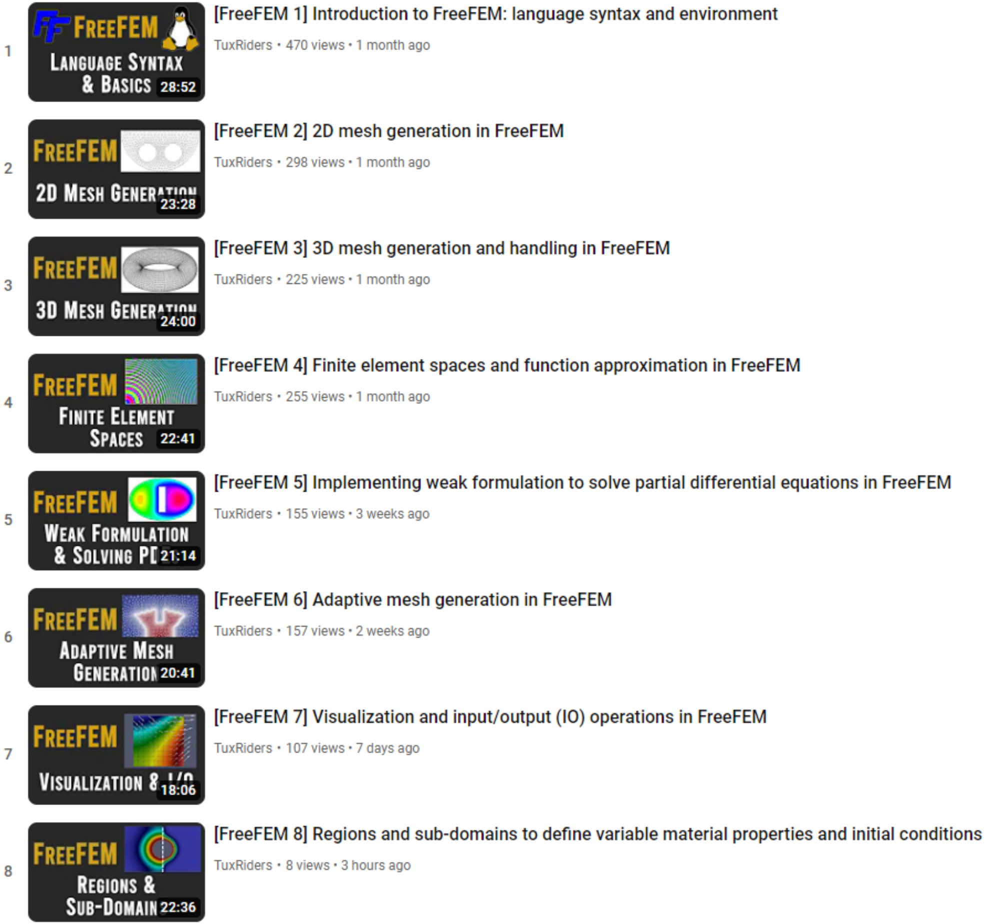
https://youtube.com/TuxRiders

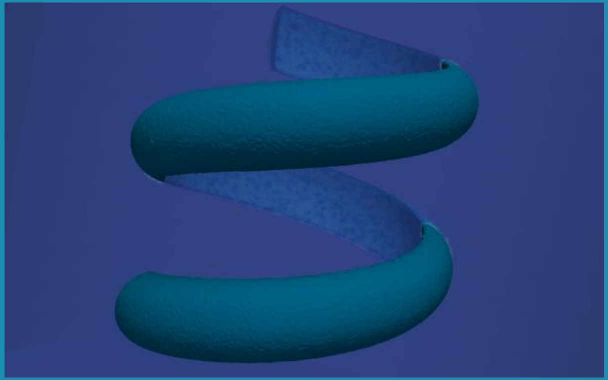


KU LEUVEN

FreeFEM Series







Thank you for your attention

https://mbarzegary.github.io

@MojBarz