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High-Performance Computing in Biomedical Engineering; a Use-case for Biomaterials Degradation Modeling

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High-Performance Computing (HPC)

- Driven by need for more computing power
- Leveraging (distributed) compute resources to solve complex problems
- Computations in parallel over lots of compute elements (software)
- Very fast network to connect compute elements (hardware)
- Why do we need HPC?
  - Complete a time-consuming operation in less time
  - Perform a high number of operations per seconds

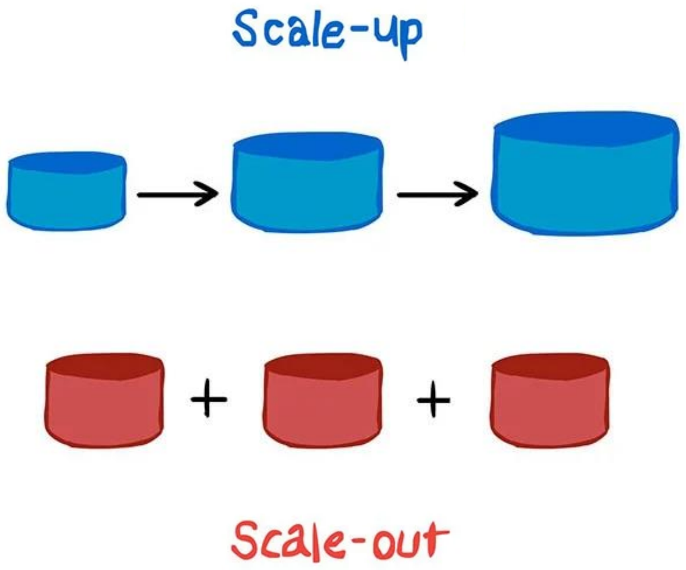
(source: tech.eu)

Typical HPC Workloads

- Physics, astrophysics
- Bioscience, genomics, bioinformatics
- Artificial intelligence
- Chemistry, molecular sciences
- Computer aided engineering
- Computer science, mathematics
- Big data analytics
- Financial and economic modeling
- Weather and climate
- Cyber security
- Advanced graphics
- …

Supercomputing in Computational Sciences

- Solving more complex problems in less time
- Scale up
  - Faster CPUs
  - Larger memories
  - More advanced hardware/software
- Scale out
  - Large parallel applications
  - Many small- to medium- size jobs



(source: turbonomic.com)

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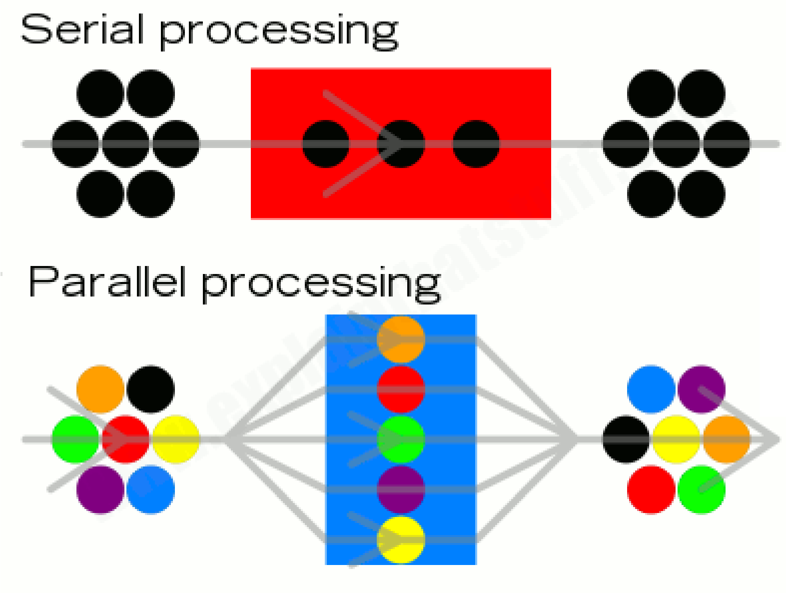
Synonymous to Parallel Computing

- Parallelism is available at many levels
- All HPC machines are parallel architectures
- Two fundamental parallel architectures:
  - Shared memory systems
  - Distributed memory systems
- Scaling benchmark matters a lot!



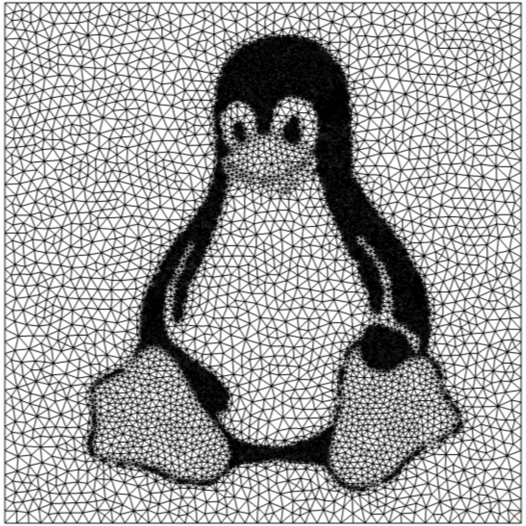
(source: explainthatstuff.com)

HPC in Biomedicine and Biomedical Engineering

- Much effort is put into model credibility and regulatory context of the simulation predictions
- Scalability of models to benefit from rapidly growing computing power
- The potential impact of HPC:
  - employing more quantities of data or parameters
  - using them to perform predictive modelling and simulation
  - in order to deliver therapies and to enhance clinical decision making
  - on time scales far shorter than those in academic research activities

Role of Free and Open Source Software

- The role that open-source movement has played is undeniable
- Freedom and flexibility in HPC
- Huge number of relevant programs and libraries
  - Operating system and system tools
  - Job scheduling and load balancing systems
  - High-performance libraries, tools, and solvers
- Most scientific contributions and codes are open-source



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Computational modeling of biodegradation behavior of degradable metals

A high-performance computing project use-case

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
- Can be solved by:
  - Mathematical modeling of biodegradation
  - Coupling biodegradation models with tissue growth models
  - Considering environmental effects

Modeling Workflow

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

→

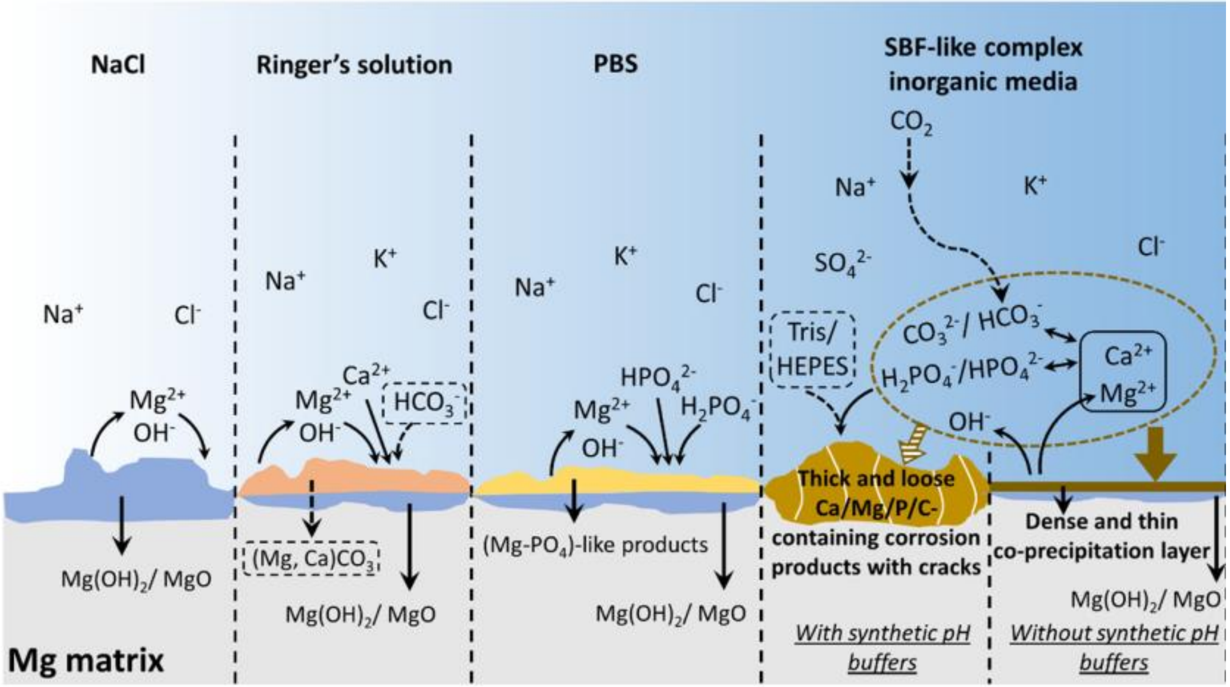
Computational Models

- 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)

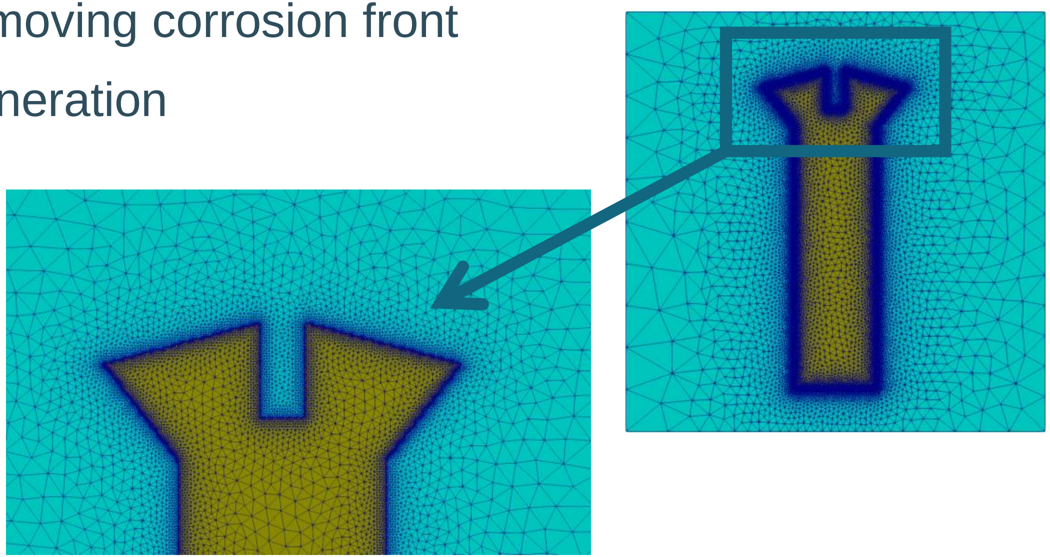
Constructing Mathematical Model

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

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

Constructing Computational Model

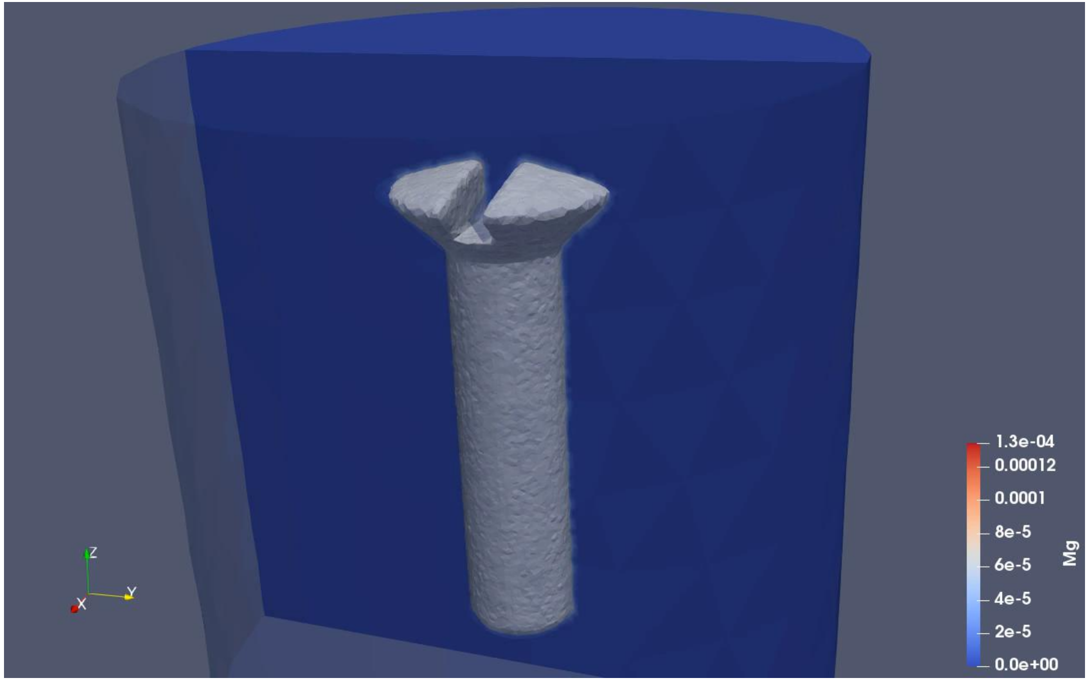
- Not feasible to implement models in sophisticated software packages
- Discretizing PDEs, finite element method
- Level-set for capturing the moving corrosion front
- Adaptively refined mesh generation



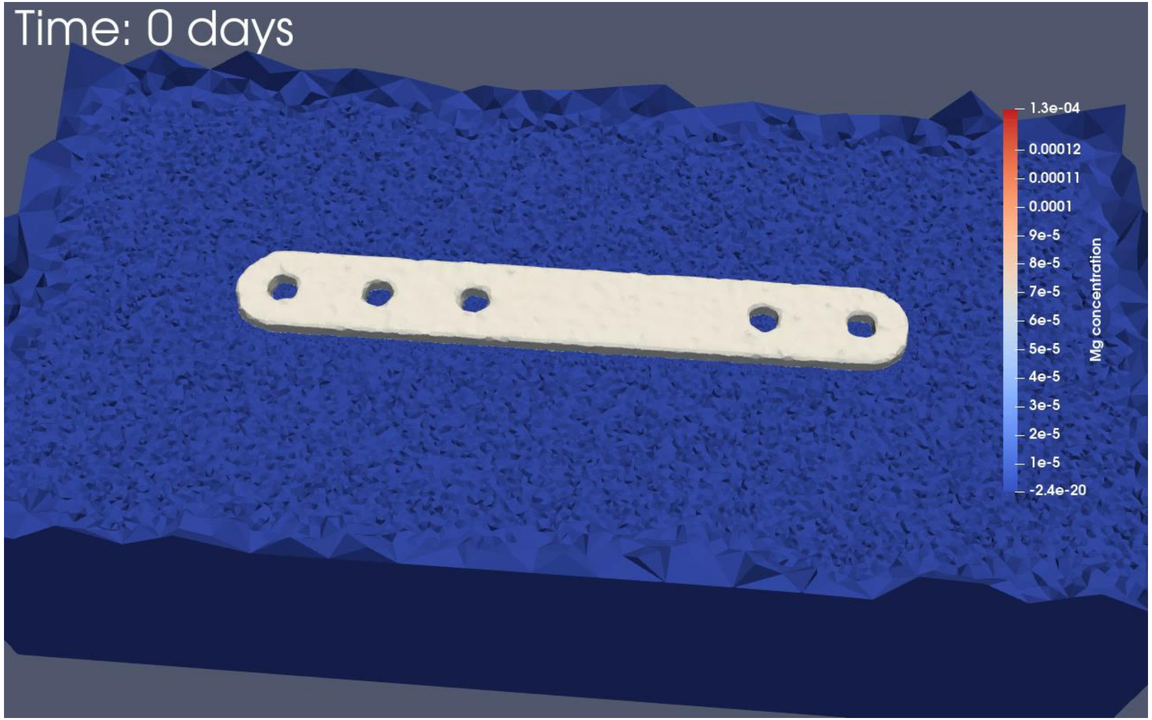
Implementing Computational Model

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

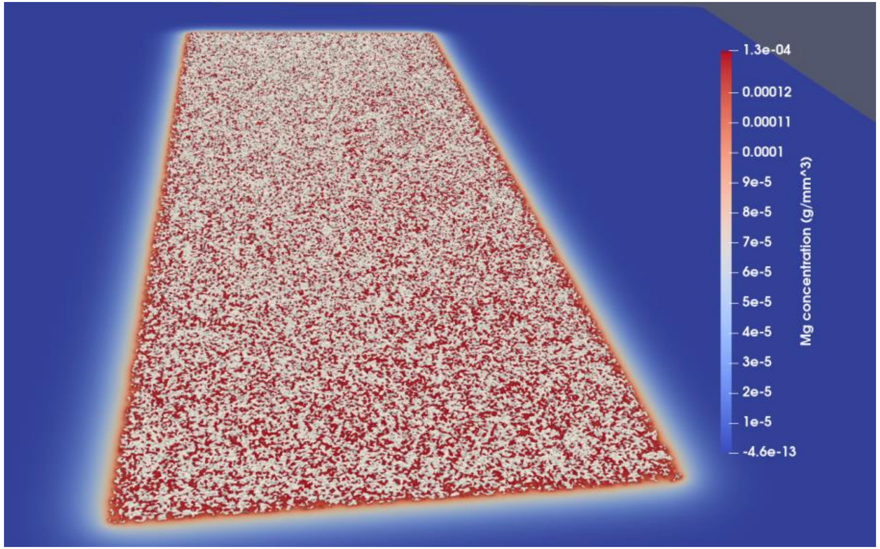
Simple Screw Degradation



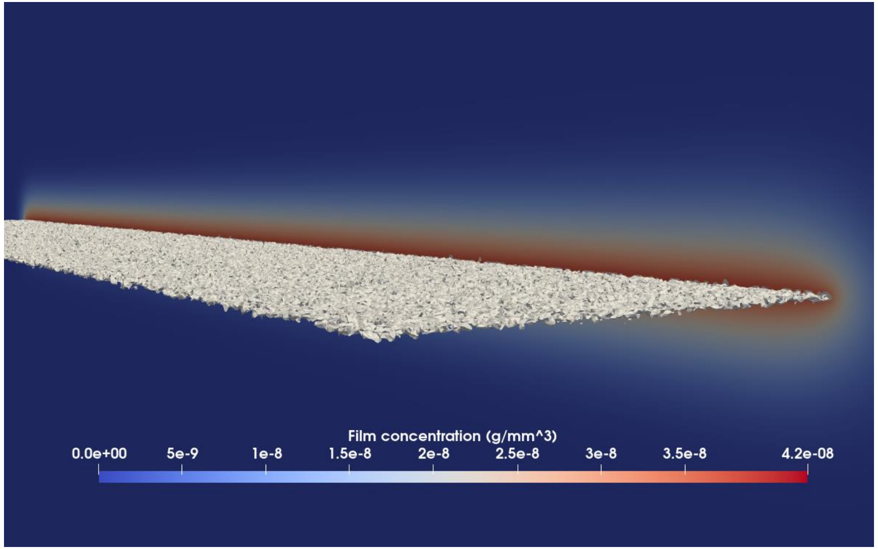
Jaw Bone Plate Degradation



Narrow Cuboid Degradation



Release of Mg ions



Formation of the protective film

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

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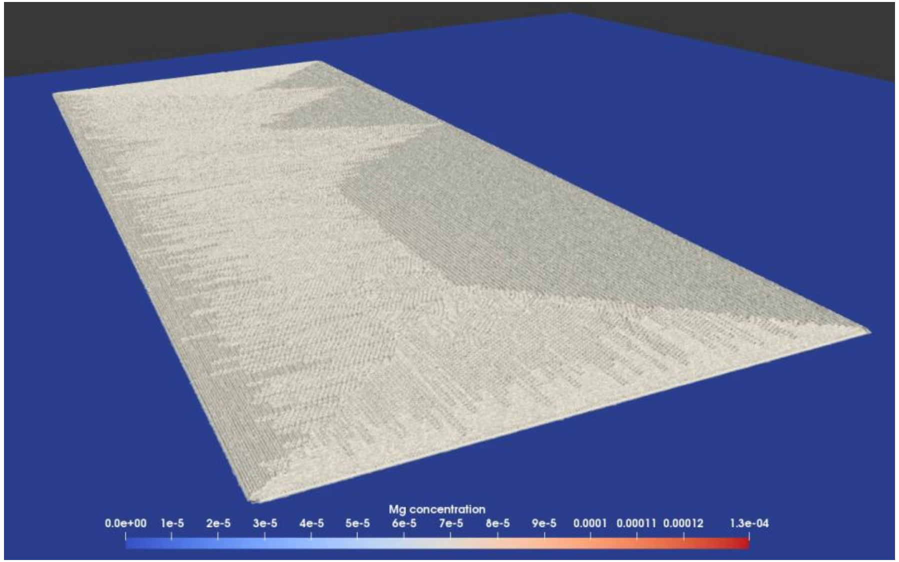
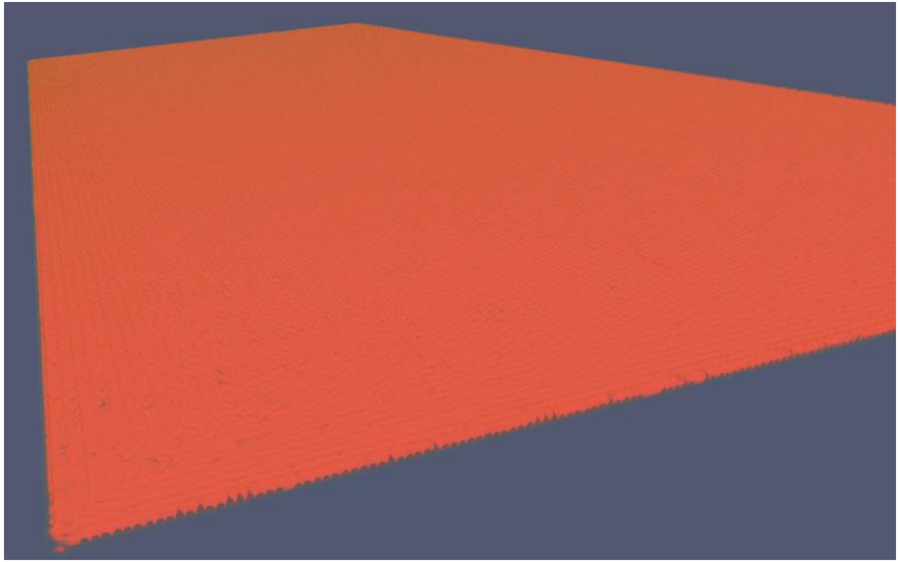
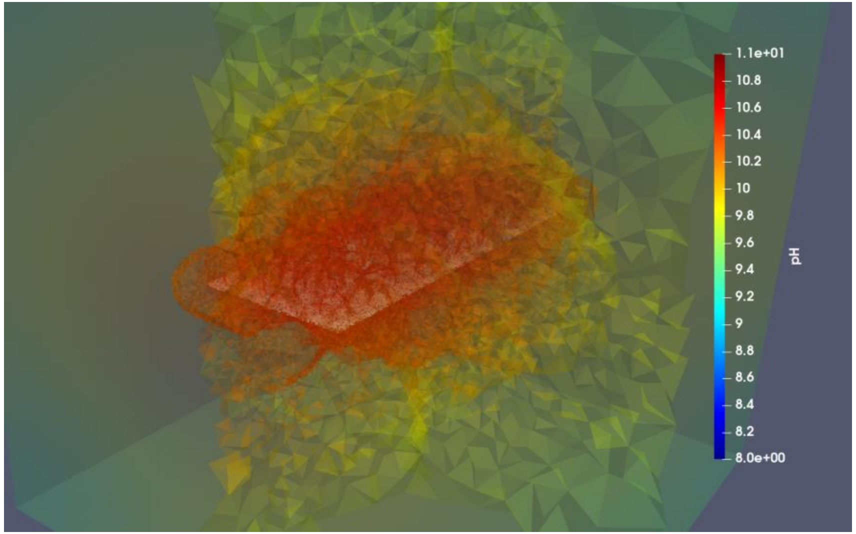
Simulation Results - Degradation



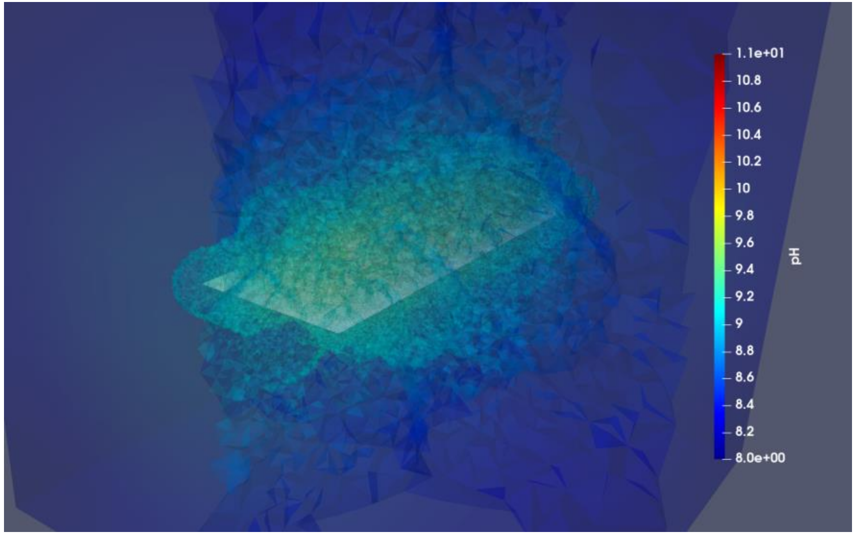


(Barzegari et al., Corrosion Science, 190, 2021)

Simulation Results - pH Change



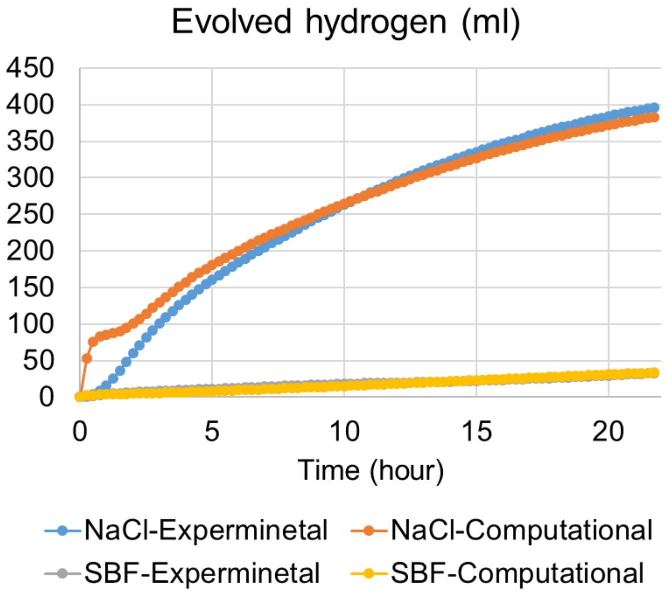
High diffusion (Saline solution)

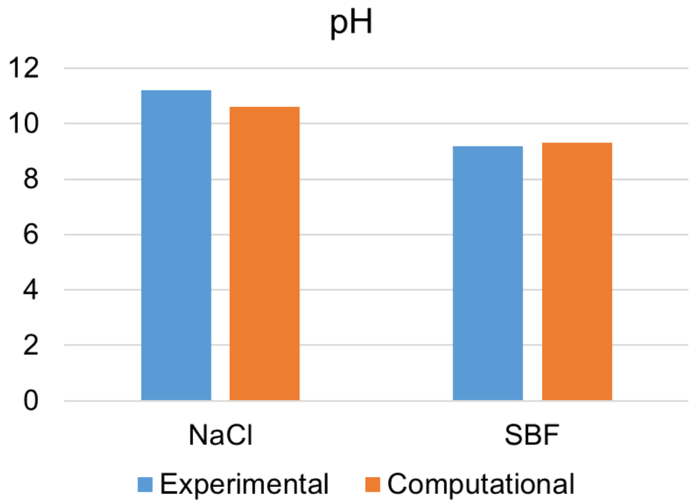


Low diffusion (Buffered solution)

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

Quantitative Results





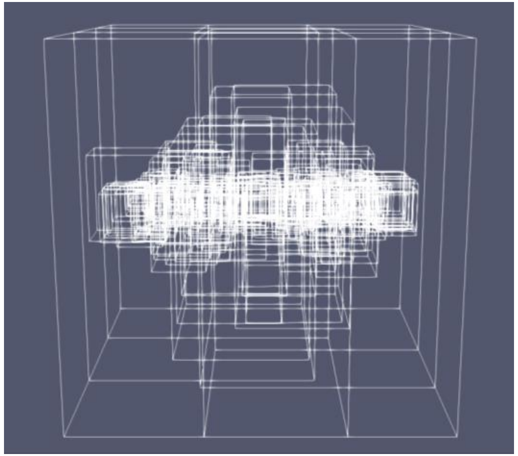
(Barzegari et al., Corrosion Science, 190, 2021)

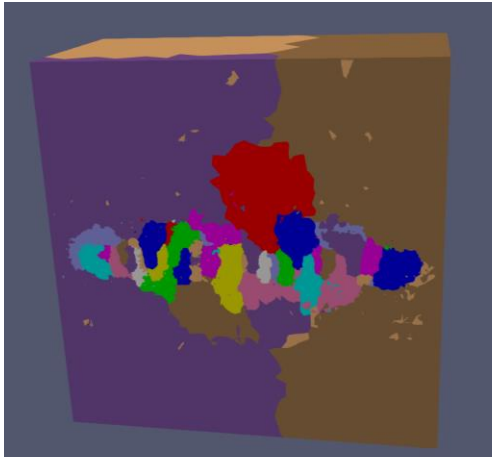
High-Performance Computing Approach

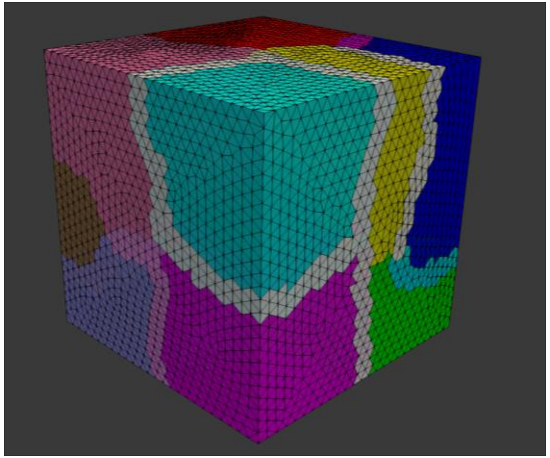
- Distributing the mesh among available resources
  - High-performance mesh decomposition
  - Overlapping Schwarz method
- Solving the linear system of equations
  - BoomerAMG preconditioner
  - GMRES iterative solver
  - Fieldsplit for fluid flow

High-performance Mesh Decomposition

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

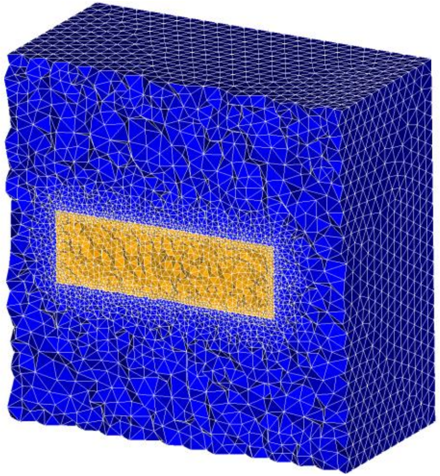


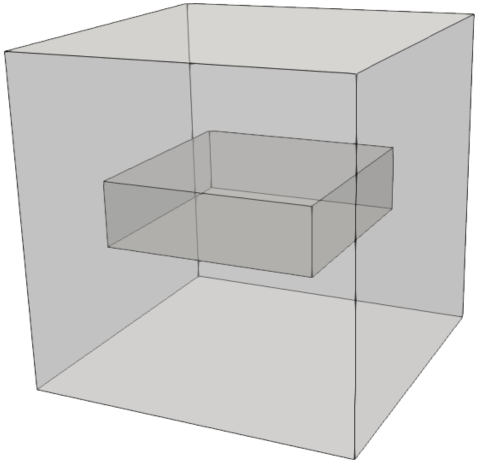




Performance Analysis

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





(Barzegari et al., International Journal of High Performance Computing Applications, 35, 2021)

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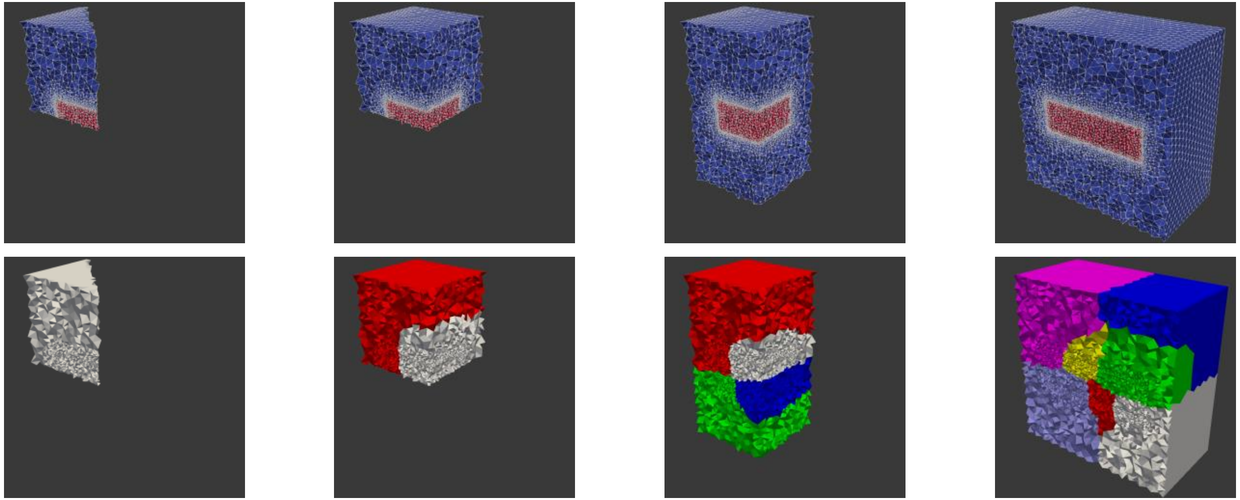
Parallelization Benchmark

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

Problem size

Mesh partitioned to available CPU cores



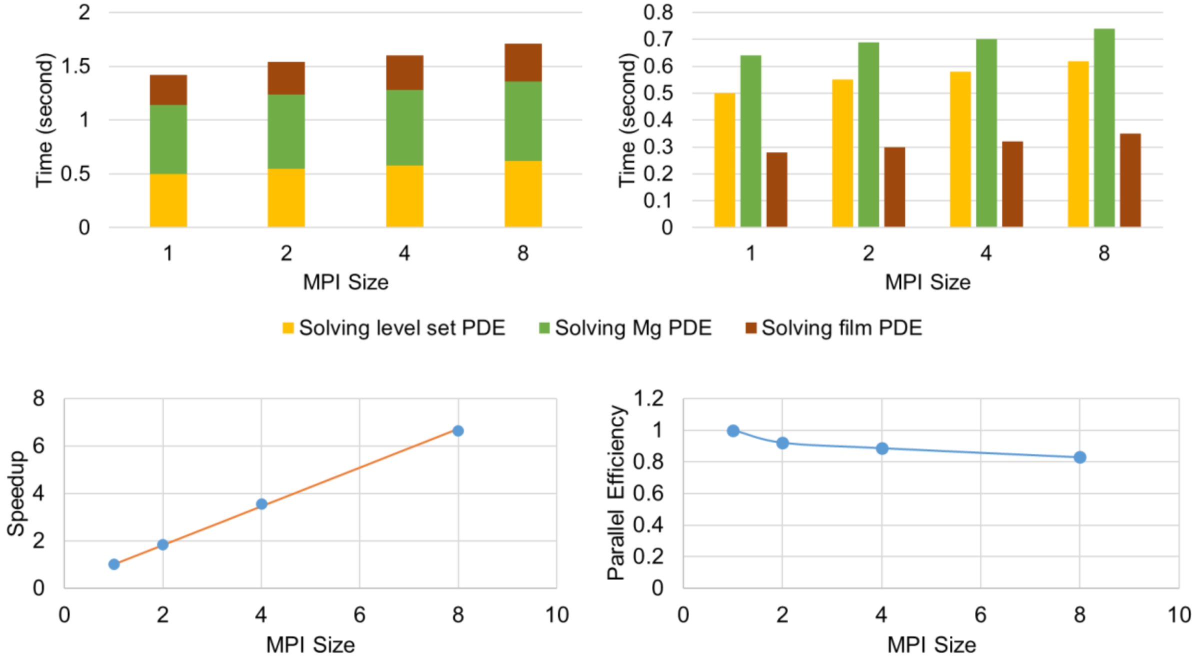
1 core 2 cores 4 cores 8 cores

Weak Scaling Analysis

Gustafson’s law

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

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



(Barzegari et al., International Journal of High Performance Computing Applications, 35, 2021)

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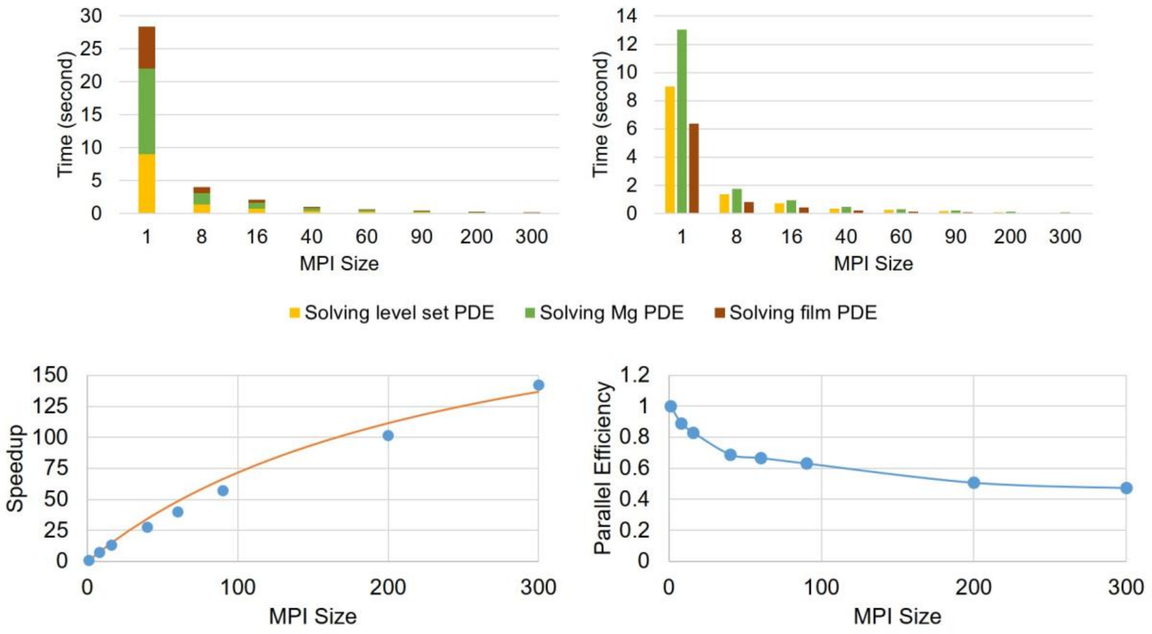
Strong Scaling Analysis

Amdahl's law

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

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



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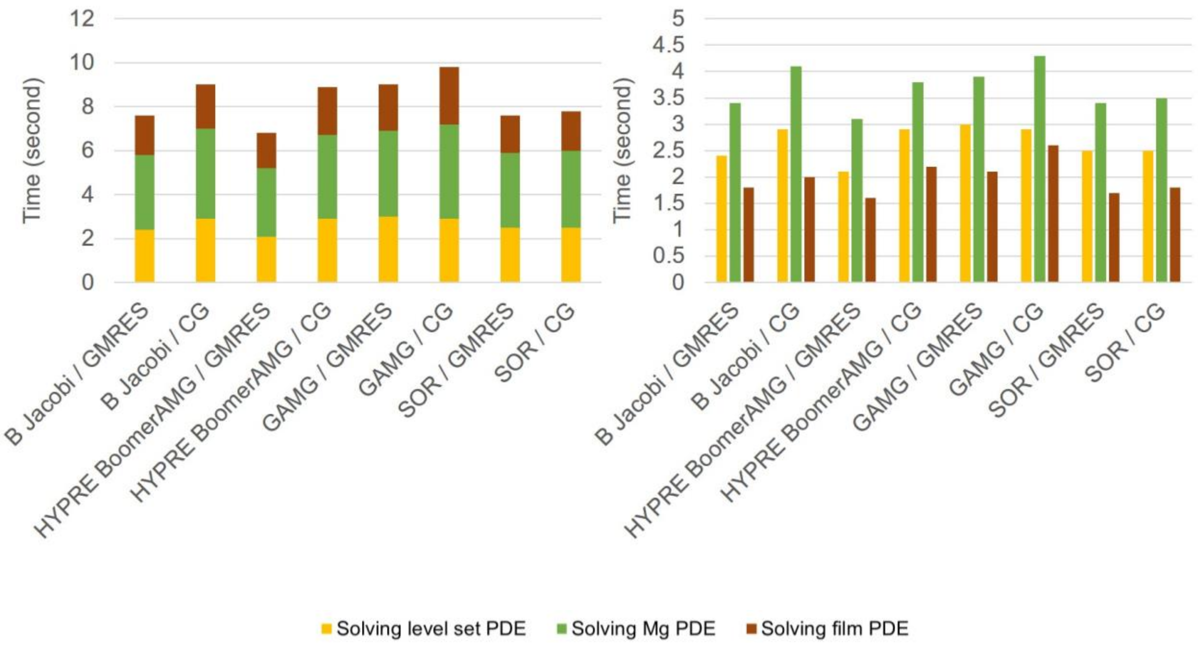
Preconditioner/Solver Performance



(Barzegari et al., International Journal of High Performance Computing Applications, 35, 2021)

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

- The importance of high-performance computing in computational modeling works in the field of biomedical engineering
- Use-case: a quantitative computational model to assess the degradation behavior of biodegradable metallic implants in-silico
- Performance evaluation tests to measure the parallel efficiency and linear scalability of the employed parallelization approaches

Thank you for your attention!

https://mbarzegary.github.io

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