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High-Performance Numerical Simulation of Biodegradation Process with Moving Boundaries

FreeFEM Days, 11th Edition

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0 Our Research Group

- Supervisor: Prof. Ir. Liesbet Geris
- Research profile:
  Computational Tissue Engineering, Computational Biomechanics, Computational Biology, Computational Genomics

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1 Outline

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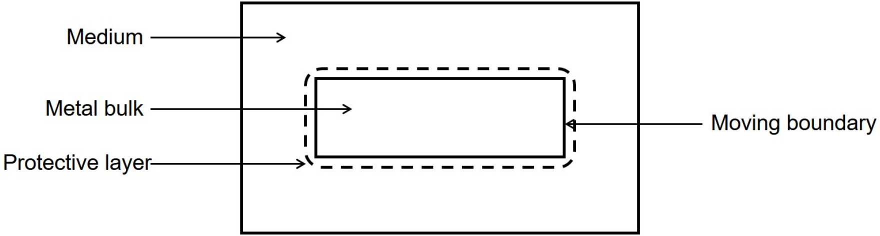
1 Reaction-Diffusion Systems with Moving Boundaries

- Stefan problems
- Diffusion-controlled interface
- Diffusion and reaction lead to the change of domain geometry
- Degradation is an example of such a system

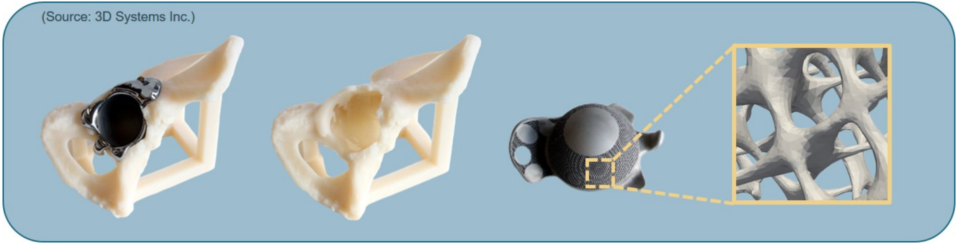
1 Biodegradation Process

- Dissolution of the bulk material
- Formation of a protective film
- Effect of ions in the medium



1 A Sample Application

- Hip joint replacement implants
- Tuning the degradation parameters to the rate of bone growth



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2 Outline

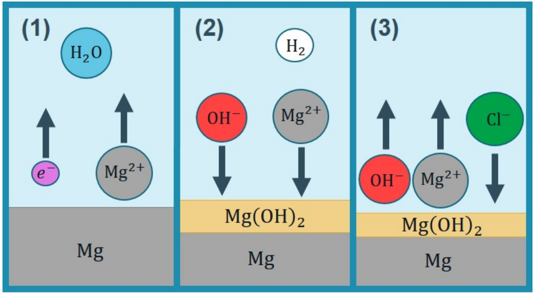
2 Chemistry of Biodegradation

Some of the chemical reactions:

$$Mg \rightarrow Mg^{2+} + 2e^-$$

$$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$$

$$Mg^{2+} + 2OH^- \xrightarrow{k_1} Mg(OH)_2$$



$$Mg(OH)_2 + 2Cl^- \xrightarrow{k_2} Mg^{2+} + 2Cl^- + 2OH^-$$

2 Reaction-Diffusion Equations

$$C_{\mathrm{Mg}} = C_{\mathrm{Mg}}(x,t), \quad C_{\mathrm{Film}} = C_{\mathrm{Film}}(x,t) \quad x \in \Omega \subset \mathbb{R}^3$$

$$\frac{\partial C_{\mathrm{Mg}}}{\partial t} = \nabla \bullet \left(D^e_{\mathrm{Mg}} \bullet \nabla C_{\mathrm{Mg}}\right) - k_1 C_{\mathrm{Mg}} \left(1 - \frac{C_{\mathrm{Film}}}{[\mathrm{Film}]_{\mathrm{max}}}\right) + k_2 C_{\mathrm{Film}} [\mathrm{Cl}]^2$$

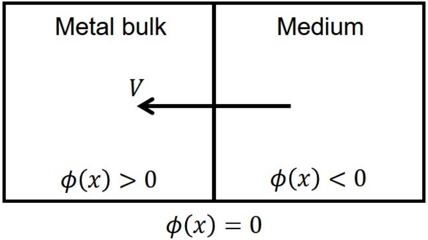
$$\frac{\partial C_{\mathrm{Film}}}{\partial t} = k_1 C_{\mathrm{Mg}} \left(1 - \frac{C_{\mathrm{Film}}}{[\mathrm{Film}]_{\mathrm{max}}}\right) - k_2 C_{\mathrm{Film}} [\mathrm{Cl}]^2$$

$$D^e_{\mathrm{Mg}} = D_{\mathrm{Mg}} \left(\left(1 - \frac{C_{\mathrm{Film}}}{[\mathrm{Film}]_{\mathrm{max}}}\right) + \frac{C_{\mathrm{Film}}}{[\mathrm{Film}]_{\mathrm{max}}} \frac{\epsilon}{\tau}\right)$$

2 Level Set Method

Implicit signed distance function $\phi = \phi(x, t) \quad x \in \Omega \subset \mathbb{R}^3$

$$\frac{\partial \phi}{\partial t} + \underbrace{\vec{V} \bullet \nabla \phi}_{\text{External velocity field}} + \underbrace{\mathrm{v}|\nabla \phi|}_{\text{Normal direction motion}} = \underbrace{b\kappa|\nabla \phi|}_{\text{Curvature - dependent term}}$$



2 Coupling Mass Transfer and Level Set

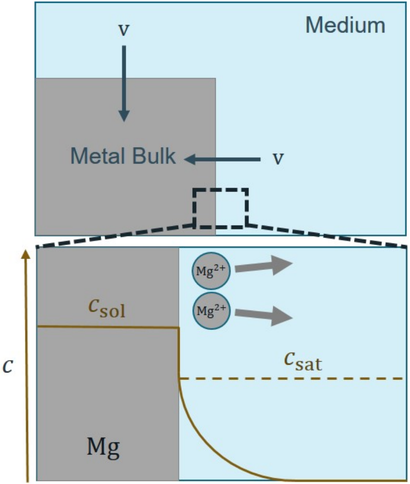
$$\frac{\partial \phi}{\partial t} + \mathrm{v}|\nabla \phi| = 0$$

Rankine-Hugoniot:

$$\{\mathbf{J}(x,t) - (c_{\mathrm{sol}} - c_{\mathrm{sat}})\,\mathrm{v}(x,t)\} \cdot n = 0$$

$$D^{e}_{\mathrm{Mg}} \nabla_n C_{\mathrm{Mg}} - ([\mathrm{Mg}]_{\mathrm{sol}} - [\mathrm{Mg}]_{\mathrm{sat}})\,\mathrm{v} = 0$$

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



3 Outline

3 Weak Formulation

Rewriting the diffusion-reaction PDE:

$$\frac{\partial u}{\partial t} = \nabla \bullet (D \bullet \nabla u) - k_1 a u + k_2 p q^2$$

Defining trial and test function space:

$$\mathcal{S}_t = \left\{ u(\mathbf{x}, t) | \mathbf{x} \in \Omega, t > 0, u(\mathbf{x}, t) \in \mathcal{H}^1(\Omega), \text{ and } \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma \right\}$$

$$\mathcal{V} = \left\{ v(\mathbf{x}) | \mathbf{x} \in \Omega, v(\mathbf{x}) \in \mathcal{H}^1(\Omega), \text{ and } v(\mathbf{x}) = 0 \text{ on } \Gamma \right\}$$

3 Weak Formulation cont.

$$\frac{\partial u}{\partial t} v = \nabla \bullet (D \bullet \nabla u) v - k_1 b u v + k_2 p q^2 v \quad \forall v \in \mathcal{V}$$

Integrate over the whole domain:

$$\int_\Omega \frac{\partial u}{\partial t} v d\omega = \int_\Omega \nabla \bullet (D \bullet \nabla u) v d\omega - \int_\Omega k_1 b u v d\omega + \int_\Omega k_2 p q^2 v d\omega$$

Integration by part, Green's divergence theory, Backward Euler scheme:

$$\int_\Omega \frac{u - u^n}{\Delta t} v d\omega = \int_\Gamma D v \bullet \frac{\partial u}{\partial n} d\gamma - \int_\Omega D \bullet \nabla u \bullet \nabla v d\omega - \int_\Omega k_1 b u v d\omega + \int_\Omega k_2 p q^2 v d\omega$$

3 Weak Formulation cont.

$$\int_\Omega uvd\omega + \int_\Omega \Delta t D \bullet \nabla \bullet u \nabla v d\omega + \int_\Omega \Delta t k_1 buvd\omega = \int_\Omega u^n vd\omega + \int_\Omega \Delta t k_2 pq^2 vd\omega$$

By defining a linear functional $(f, v) = \int_\Omega fvd\omega$

$$(u, v)[1 + \Delta t k_1 b] + \Delta t(D\nabla u, \nabla v) = (u^n, v) + \Delta t\,(f^n, v)$$

multiplying to a new coefficient $\alpha = \frac{1}{1+\Delta t k_1 b}$

$$(u, v) + \alpha\Delta t(D\nabla u, \nabla v) = \alpha\,(u^n, v) + \alpha\Delta t\,(f^n, v)$$

3 Discretization Scheme

$$\mathcal{V}_h = \operatorname{span}\left(\{\psi_i\}_{i\in\mathcal{I}_s}\right) \quad \mathcal{I}_s = \{0,\dots,N\}$$

Using 1st order Lagrange polynomials as basis functions

$$u = \sum_{j=0}^{N} c_j \psi_j(\boldsymbol{x}), \quad u^n = \sum_{j=0}^{N} c_j^n \psi_j(\boldsymbol{x})$$

$$\sum_{j=0}^{N} (\psi_i, \psi_j)\, c_j + \alpha\Delta t \sum_{j=0}^{N} (\nabla\psi_i, D\nabla\psi_j)\, c_j = \sum_{j=0}^{N} (\psi_i, \psi_j)\, c_j^n + \Delta t\, (f^n, \psi_i)$$

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3 Discretization Scheme cont.

A linear system of equations

$$\sum_j A_{i,j} c_j = b_i$$

$$A_{i,j} = (\psi_i, \psi_j) + \alpha \Delta t \left(\nabla \psi_i, D \nabla \psi_j \right)$$

$$b_i = \sum_{j=0}^{N} \alpha \left(\psi_i, \psi_j \right) c_j^n + \alpha \Delta t \left(f^n, \psi_i \right)$$

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3 Discretization Scheme cont.

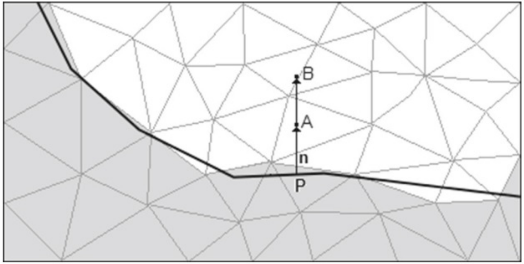
Final form as implemented in FreeFEM

$$(M + \alpha \Delta t K)c = \alpha M c_1 + \alpha \Delta t f$$

$$\begin{aligned}
M &= \{M_{i,j}\}\,, \quad M_{i,j} = (\psi_i, \psi_j)\,, \quad i,j \in \mathcal{I}_s \\
K &= \{K_{i,j}\}\,, \quad K_{i,j} = (\nabla \psi_i, D \nabla \psi_j)\,, \quad i,j \in \mathcal{I}_s \\
f &= \{f_i\}\,, \quad f_i = (f(\boldsymbol{x}, t_n)\,, \psi_i)\,, \quad i \in \mathcal{I}_s \\
c &= \{c_i\}\,, \quad i \in \mathcal{I}_s \\
c_1 &= \{c_i^n\}\,, \quad i \in \mathcal{I}_s
\end{aligned}$$

3 Level Set Implementation

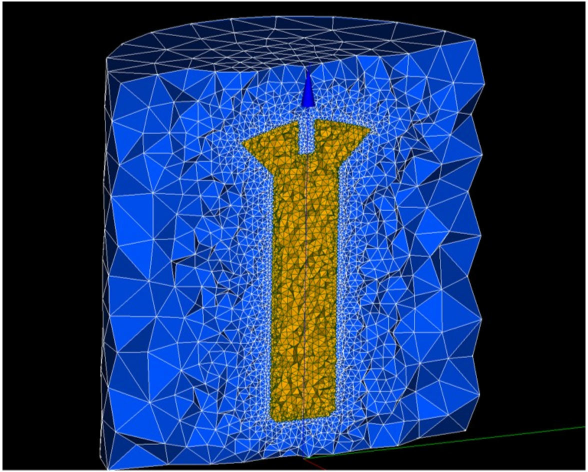
- Penalization for interface BCs
- Computing $\nabla_n C_{\mathrm{Mg}}$ correctly
- Problem of oscillation
- Too flat or too steep gradients
- Nightmare of re-distancing



(P. Bajger et al. 2017)

3 Computational Mesh

- Eulerian mesh
- Generated using Netgen in SALOME platform
- Adaptively refined on the moving interface

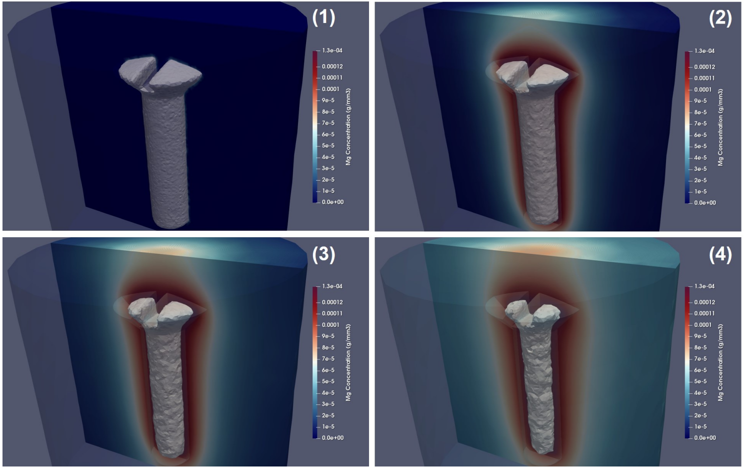


3 Parallelization

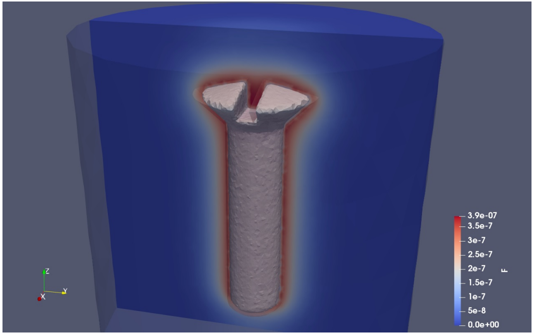
- Message Passing Interface
- Distributed numerical integration
  (assigning a number in the range of [0, MPI Size-1] to each element)
- MUMPS multifrontal direct solver

4 Outline

4 Release of Ions and Degradation - Simple Screw

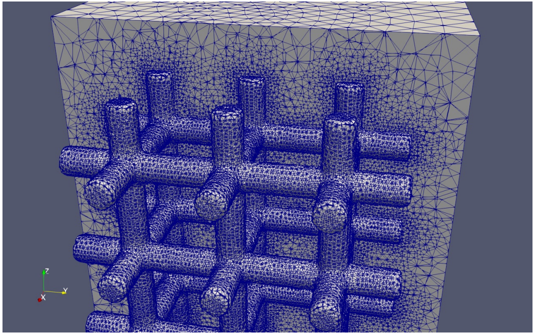


4 Film Formation - Simple Screw

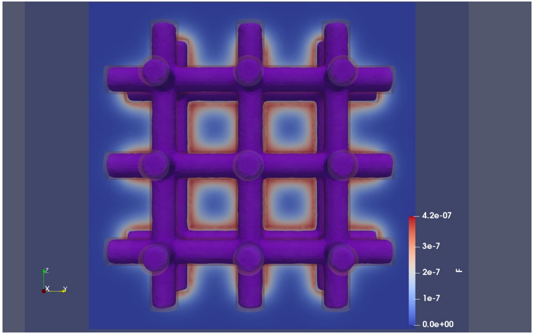


Formation of the protective film on the interface of material-medium

4 Release of Ions and Degradation - Porous Structure



Trimmed view of the computational mesh



Formation of the protective film

4 Quantitative Results

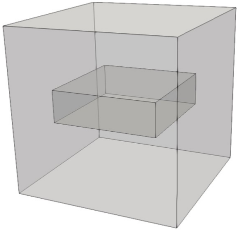
Measuring mass loss:

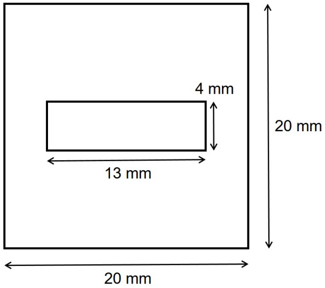
- Direct weight reduction
- Side products evolution

Using level set output for calculating mass loss

$$\mathrm{Mg}_{\mathrm{lost}} = \int_{\Omega_+(t)} \mathrm{Mg}_{\mathrm{solid}} \mathrm{d}V - \int_{\Omega_+(0)} \mathrm{Mg}_{\mathrm{solid}} \mathrm{d}V_0$$

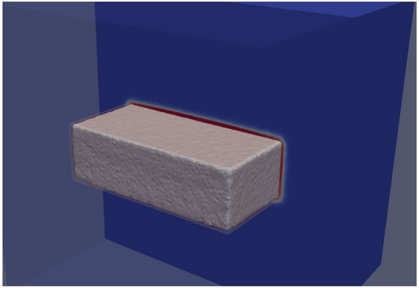
$$\Omega_+(t) = \{\mathbf{x} : \phi(\mathbf{x}, t) \geq 0\}$$

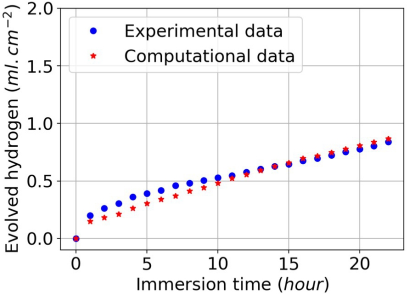




Simulation and experimental setup

4 Mass Loss and Evolving Side Products





Film formation and the comparison of predicted and experimental mass loss, measured by the evolved hydrogen gas

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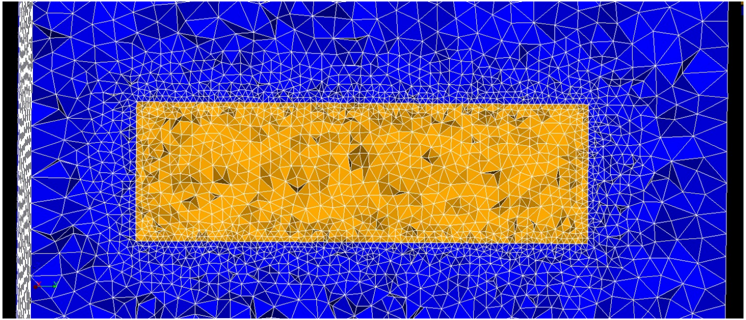
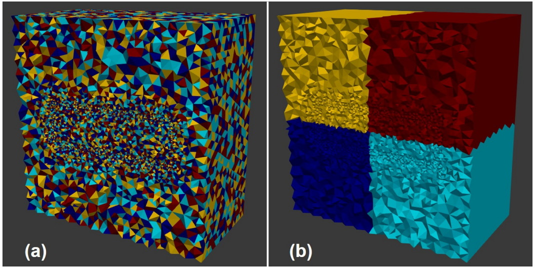
5 Outline

5 Problem Size

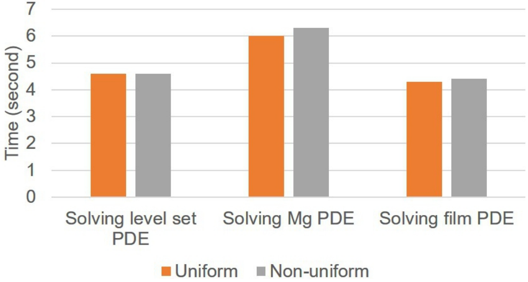
- Same setup as the model for calibration and validation
- DOF: 144k
- Elements: 831k (P1)



5 Domain Decomposition

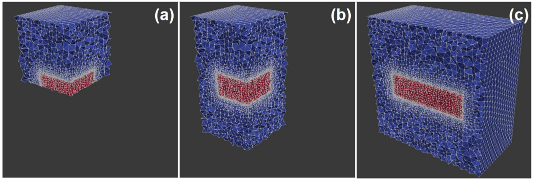


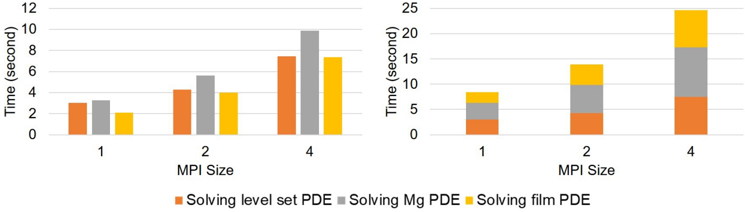
Two different approaches for domain decomposition. Colors show different mesh regions assigned to different MPI cores.



Execution time per time step

5 Weak-Scaling Test Results





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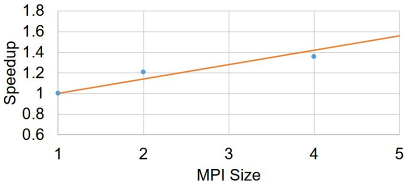
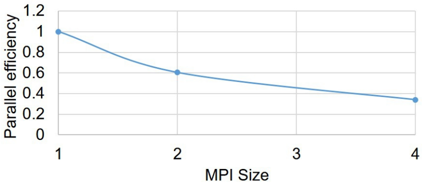
5 Weak-Scaling Test Analysis

Based on Gustafson's law:

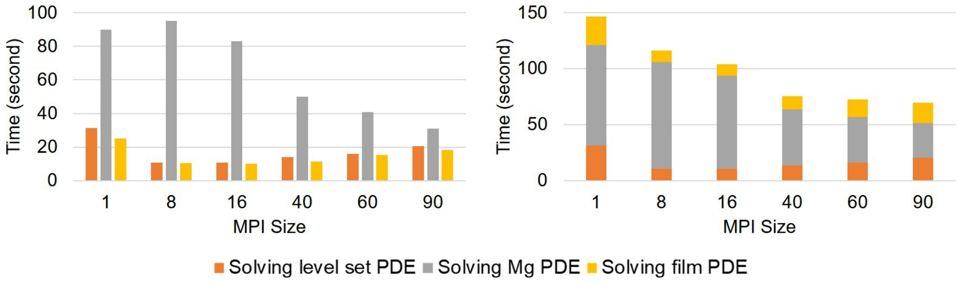
$$\text{Speedup} = f + (1 - f) \times N$$

Serial proportion $=$ 86%, Parallelizable proportion $=$ 14%





5 Strong-Scaling Test Results



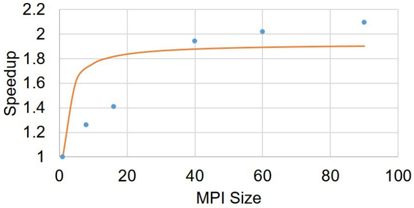
Time required to solve each PDE in each time step

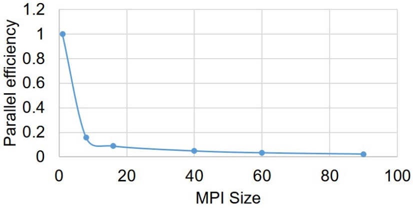
5 Strong-Scaling Test Analysis

Based on Amdahl's law:

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

Serial proportion = 52%, Parallelizable proportion = 48%





5 Conclusion

- A quantitative mathematical model and its corresponding computational model to assess the degradation behavior of biodegradable materials
- Using level set method to track the moving corrosion front during degradation
- Once fully validated, the model will be an important tool to find the right design and properties of the metallic biomaterials and implants

Thank you for your attention

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