BioDeg: corrosion/biodegradation simulation software for metallic biomaterials based on FreeFEM/PETSc/Qt

Mojtaba Barzegari, Liesbet Geris

Biomechanics Section, Department of Mechanical Engineering, KU Leuven, Leuven, Belgium

BioDeg is an open-source software written in FreeFEM, Python, and C++ for modeling the degradation of metallic biomaterials and simulating the biodegradation behavior of medical devices, implants, and scaffolds in corrosion experiments. The underlying mathematical and computational models have already been validated by comparing the predictions made by the code with the experimentally obtained quantities [1]. BioDeg supports simulating the change of morphology of the material block/implant/scaffold, release of materials, formation of surface corrosion products, the effect of the surrounding environment (such as various electrolyte solutions and chemical components as well as the presence of fluid flow), and change of experimental quantities (such as pH). It features command-line and graphical interfaces (developed using Qt), being available on all major operating systems and platforms.

BioDeg is built upon a mechanistic formulation of the biodegradation process [1]. This has been accomplished by deriving a system of time-dependent reaction-diffusion-convection partial differential equations (PDEs) from the underlying oxidation-reduction reactions coupled with Navier-Stokes equations for the fluid flow of the solution. The level set formalism was employed to track the biodegradation interface between the biomaterial and its surroundings. The equations were solved implicitly using the finite element method for spatial terms and the backward-Euler finite difference method for temporal terms on an Eulerian mesh, implemented in FreeFEM [2].

Biodegradation simulations in BioDeg can become complex and resource-demanding due to the refined mesh on the metal-electrolyte interface, which is required to increase the accuracy of employed numerical schemes to track the moving corrosion front. This expensive computational model makes it crucial to employ high-performance computing (HPC) techniques to scale the simulations to hundreds or thousands of computing nodes and decrease the simulation execution time. To this end, a high-performance domain decomposition approach was employed to partition the mesh and distribute the workload to available computing resources [3]. Additionally, efficient preconditioners and solvers, available via the rich PETSc library, were used to solve the linear system of equations resulting from the finite element discretization. The scaling tests and related benchmarks on the efficiency of this model have already been published [4].

REFERENCES

[1] M. Barzegari et al. (2021) Computational modeling of degradation process of biodegradable magnesium biomaterials. Corrosion Science 190.

[2] F. Hecht (2012) New development in FreeFem++. Journal of Numerical Mathematics 20:251–265

[3] V. Dolean et al. (2015) An Introduction to Domain Decomposition Methods. SIAM publications.

[4] M. Barzegari et al. (2021) Highly scalable numerical simulation of coupled reaction-diffusion systems with moving interfaces. The International Journal of High Performance Computing Applications 35.