High-performance numerical simulation of biodegradation process with moving boundaries

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In my PhD study, I have developed a quantitative mathematical model to predict the biodegradation of metallic biomaterials. Magnesium (Mg) has been selected to start with due to its acceptable mechanical properties, biocompatibility, and contribution in osteoinductivity [1]. The developed model captures the release of Mg ions, the formation of a protective film that slows down the degradation rate, and the dissolution of this film due to the effect of some ions in the surrounding fluid. This has been accomplished by deriving a system of time-dependent reaction-diffusion PDEs from the underlying oxidation-reduction reactions. The interface between the metal and its surroundings moves due to the loss of material, so the Level Set formalism has been employed to track the biodegradation front. The equations were solved implicitly using the finite element method for spatial terms and backward-Euler finite difference method for temporal terms on an Eulerian mesh. The mesh has been refined adaptively on the interface to increase the numerical accuracy of the simulated model. In order to increase performance and efficiency, the code has been developed in a way that can be distributed across several computational nodes using high-performance computing (HPC) techniques. The code is implemented in FreeFEM [2] and uses Message Passing Interface (MPI) to parallelize numerical integration on the investigated mesh. It also uses MUMPS distributed solver to solve the derived system of algebraic equations. A typical 3D biodegradation simulation usually consists of 800,000 elements and a DOF of 200,000 for each PDE, approximately.

REFERENCES

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[2] F. Hecht (2012) New development in FreeFem++. J Numer Math 20:251–265