High-performance computing in biomedical engineering; a use-case for biomaterials degradation modeling

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Abstract: The use of computational modeling in medical-related studies has risen exponentially in recent years, and more reliable developed models are being released each year for various sub-fields of this domain. One of the hurdles to accelerate the uptake of said models into clinical practice is that of scalability of the developed codes and models to benefit from rapidly growing computing power and advancements in hardware resources. This has received less attention thus far, but having scalable models that use the available computing resources more efficiently allows constructing more comprehensive models that capture more realistic phenomena, leading to more accurate simulations and predictions. Taking advantage of high-performance computing (HPC) techniques can help the field to move towards more reliable and accurate computational models for personalized medicine. As relevant examples in the tissue engineering field, we have developed a set of high-performance computational models to predict the rate of degradation for biodegradable metallic implants as well as neotissue growth for bone tissue engineering applications.

In order to take advantage of biodegradable metallic materials (magnesium, zinc, and iron) in tissue engineering applications, their degradation parameters should be tuned to the rate of regeneration of new tissue. To this end, we have developed a mathematical and computational model to predict the biodegradation behavior of these materials. Our developed model captures the release of metallic ions, changes in pH, the formation of a protective film, the elimination of this film in presence of different ions, and the effect of perfusion of the surrounding fluid. This has been accomplished by deriving a system of time-dependent reaction-diffusion-convection partial differential equations from the underlying oxidation-reduction reactions and solving them using the finite element method. The level set formalism was employed to track the biodegradation interface between the biomaterial and its surroundings, but tracking the moving front at the diffusion interface requires high numerical accuracy of the diffusive state variables, which was achieved using a refined computational grid. This made the model computationally intensive and in need of parallelization. Thus, a parallelization approach was also implemented using high-performance domain decomposition and high-performance preconditioners/solvers to enable the model to simulate large-scale systems with high efficiency in HPC environments. The weak-scaling and strong-scaling tests were performed to evaluate the performance of the parallelized algorithm, showing a proper scaling for hundreds of cores.

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