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Massively parallel finite element simulation of reaction-diffusion systems with moving boundaries: a use-case for biomaterials degradation modeling

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Moving-boundary problems [1] are a subset of the general concept of boundary-value problems which not only require the solution of the underlying partial differential equation (PDE), but also the determination of the boundary of the domain (or sub-domains) as part of the solution. This approach can be used to model a plethora of phenomena ranging from phase separation and multiphase flows in materials engineering to bone development and tumor growth in biology. Reaction-diffusion systems are the mathematical models in which the change of state variables occurs via transformation and spreading. These systems are described by a set of parabolic PDEs and can model a large number of different systems in science and engineering. Combining the reaction-diffusion systems with moving-boundary problems provides a way to study the systems in which the diffusion and reaction lead to the change of domain geometry. Such systems have great importance in various real-world scenarios in chemistry and chemical engineering as well as environmental and life sciences.

In this study, the material degradation phenomenon has been investigated as an example of a reaction-diffusion system with moving boundaries, in which the loss of material due to corrosion leads to movement of the interface of the bulk material and surrounding corrosion environment. More specifically, the degradation of magnesium (Mg) in simulated body fluid has been chosen as a case study. Magnesium has been chosen due to its growing usability as a degradable material in biomedicine, where it is usually used in biodegradable implants for bone tissue engineering and cardiovascular applications [2, 3].

In the current study, we developed a mechanistic model of the material degradation process by constructing a mathematical and computational model to predict the biodegradation behavior. The 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 movement of the corrosion front. This has been accomplished by deriving a system of time-dependent reaction-diffusion PDEs 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. Improving the accuracy requires a refined computational mesh, leading to a more computation-intensive simulation. To overcome this challenge and yield more interactable simulations, scalable parallelization techniques were

implemented, making the model capable of being run on massively parallel systems to reduce the simulation time. It is also worth noting that in a real-world application, such systems require a calibration (also called parameter estimation or inverse problem), in which the model should be simulated hundreds of times. This makes the parallelization even more crucial for these models.

The model was implemented in FreeFEM [4], an open-source PDE solver to facilitate converting the weak formulation of the finite element scheme to a linear system $Ax = b$. For parallelization, a restricted additive Schwarz method for domain decomposition was employed to split the mesh into smaller domains such that the global solution of the linear system is achieved by solving the problem on each smaller local mesh. In order to yield the highest performance for solving the equations, an iterative approach using the Krylov subspaces (KSP) method was employed, in which we preconditioned the equation using a proper preconditioner and then solved it with an iterative solver. A variety of different combinations of KSP types and preconditioners, available via the PETSc library were evaluated, out of which the best performance for the reaction-diffusion system model was achieved using the HYPRE BoomerAMG preconditioner and the GMRES solver.

The degradation data to validate the model was collected from corrosion tests of Mg. The model parameters were calibrated using a Bayesian optimization approach, and the obtained parameters were used to simulate the pH changes in saline and buffered solutions. The results demonstrate the capability of the model to capture the degradation interface movement and to mimic the underlying chemical phenomena since the predicted mass loss and pH changes were in line with the experimentally obtained values. More details of this can be found in our recently published work [5]. To evaluate the performance of the implemented parallelism, a set of weak and strong scaling tests (using 1, 8, 16, 40, 60, 90, 200, and 300 MPI cores) was performed, showing a proper scaling for hundreds of cores. By fitting Gustafson's and Amdahl's laws on the scaling test results, the maximum parallelizable portion of the code was calculated to be 82% and 99% for the weak-scaling and strong-scaling tests, respectively, which is a reasonable theoretical scaling for both cases.

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