Four years of scientific computing using FreeFEM in the field of computational biomedical engineering

Mojtaba Barzegari, Laura Lafuente-Gracia, Liesbet Geris

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

Over the past four years, the open-source finite element solver FreeFEM has been extensively used in the computational biomechanics research unit (http://www.biomech.ulg.ac.be/) for a wide range of simulations and modeling studies in the field of computational biomedical engineering and *in silico* medicine. FreeFEM integration with a couple of powerful scientific computing tools and libraries, such as PETSc, HPDDM, Mmg (and ParMmg), Tetgen, METIS (and ParMETIS), SCOTCH, etc., allowed us to take advantage of this open-source domain-specific language efficiently in the development of multiple types of computational models. This benefit has been boosted by the available features to work with various mesh formats, allowing us to use FreeFEM codes in different stages of our modeling workflows.

In this talk, a brief overview of the following carried out research works, with FreeFEM being part of the modeling workflow, will be presented:

- Computational modeling of the biodegradation process of metallic biomaterials, developed by
 deriving a system of time-dependent reaction-diffusion-convection PDEs coupled with NavierStokes equations for hydrodynamics conditions and a level-set formalism for tracking the
 morphological changes.
- BioDeg, an open-source software written in FreeFEM, Python, and C++ for simulating the degradation behavior of medical devices, built on top of the biodegradation model with a cross-platform user interface developed using Qt.
- Tissue growth models, in which the growth of newly formed tissue in various processes were modeled using moving boundary approaches and interface tracking methods, implemented using both the phase-field and level-set methods in 2D and 3D.
- Bone fracture healing models, where a system of non-linear taxis-diffusion-reaction PDEs
 describing the spatiotemporal evolution of biochemical factors, cells, and tissues was derived
 and coupled with discrete representation of blood vessels for simulating bone regeneration.
- Pancreatic cells viability, a time-dependent reaction-diffusion model to investigate whether groups of cells can survive in various conditions prior to transplantation.
- Geometry construction and mesh generation for various open-porous tissue engineering scaffolds created based on TPMS lattice infills.
- Integrating topology optimization approaches with biodegradation models to simulate the mechanical integrity of infilled structures for medical applications.
- Building a structural analysis component for open-source software TFMLab, a traction-force microscopy code to compute active cellular forces.
- A case study demonstrating HPC approaches: modeling the degradation behavior of a stiffness-optimized patient-specific porous implant, leading to a computational model with 46M elements simulated using 2K CPU cores, with scaling tests being performed on MPI sizes of 2K-8K.