Development of a new and efficient adaptive phase field method: application to the prediction of patient-specific bone remodeling

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In order to adapt to the external loadings and maintain its mechanical performance, bone undergoes a continuous renewal process called remodeling. Mechanical loading controls the bone mass and structure, where different cells are involved, but where mechanico-sensing cells called osteocytes have a primal role. The chemical signal induced by the osteocytes controls two competing cells: osteoclasts that lead to bone resorbtion and osteoblasts which deposit bone. The understanding of this mechano-biological system is of prime importance to understand how the bone microstructure evolves in the ostheoporosis context for instance. Various modeling and numerical approaches have been developed to tackle this scientific challenge in a patient-specific context, like voxel-based methods for instance. These methods can tackle both the complex geometry of the bone and its evolution. Unfortunately, they are not efficient from a computational point of view. To overcome efficiency issues, phase field models have been developed, based on a diffuse interface approach and have been used to compute the mechanical properties of trabecular bone structures. With this approach, the interface is modeled with a finite thickness, and the computational domain is constituted of the bone and surrounding tissue. The smaller this thickness lengthscale, the closer the results are to a sharp interface solution. Mesh adaptation is necessary to resolve the fields at this lengthscale at a reasonable cost, but work done until now provides results in very small domains.

The purpose of this PhD to develop numerical strategies that improve (even more) the efficiency of phase field methods for such applications, while keeping the *specific-patient* context. For that, several steps are foreseen within this work:

1) *implement a phase field finite element solver* (based on previous work done on phase field and modified level-set solvers at ICI, and implemented within ICI-tech - ICI's parallel scientific computing library) from a biological model established for bone remodeling, that shall be coupled the multiphase mechanical problem solver
2) *reduce the computational cost by developing automatic adaptive strategy techniques, coupled to parallel computing*
   At ICI, finite element solvers, like the ones cited in 1), are developed combining p-adaptation (high order interpolations) and h-adaptation (automatic mesh refinement) techniques, already present in ICItech. However, phase field models require using very small time steps since thickness required to model the diffuse interface must be very small (to approach the real sharp interface) due to curvature dependent velocity of propagation, for example. First objective is to develop, within ICI-tech, a *t-adaptation* method to be able to increase mesh sizes and time steps, and thus reduce largely the computational time. This shall be done by developing new space-time error estimators on the solution fields that will give us the good space-time metrics field, used by ICI's automatic anisotropic parallel mesher
3) *integrate the developments in a patient-specific context*. For that, computational domains shall be mapped from patient images but not by using a classical voxel-approach, but by interpolating directly the image in the mesh and by using developments on mesh adaptation to attain the required accuracy. Complexity of shapes and patient dedicated morphologies

requires computations at very large scale and usage of high performance computing techniques and resources, even with a full parallel programming framework and the improvements of points 1) and 2). AI (artificial intelligence) techniques for shape parametrization are developed at ICI for other medical applications and can also be reused in this context to obtain, in a faster and efficient way, computational domain's configuration for a specific patient

4) *application to trabecular bone remodelling*. Validation of the code can be performed using literature benchmarks, but verification of the developments will be done on images from real patients, by comparing the temporal numerical and real (imaging) evolutions of their bone structure. This part of the work may be done in collaboration with colleagues from CHU Nantes (University Hospital in Nantes).

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Skills required: knowledge on approximation methods for PDEs (like finite elements), experience on programming for scientific applications (C++ would be perfect!), parallel computing (a real +!)

Bibliography

[1] Aland S, Stenger F, Müller R, Deutsch A, Voigt A. A Phase Field Approach to Trabecular Bone Remodeling. Front. Appl. Math. Stat. (2020)| https://doi.org/10.3389/fams.2020.00012

[2] Aland S, Landsberg C, Müller R, Bobeth M, Langheinrich AC, Voigt A. Adaptive diffuse domain approach for calculating mechanically induced deformation of trabecular bone. Comput Meth Biomech Biomed Eng. (2014) 17:31–8. doi: 10.1080/10255842.2012.654606