Postdoc position

Project title: Drug Release from Capsules Induced by Acoustic Stimulation: A numerical study

Host laboratory: Laboratoire Biomécanique et Bioingénierie (UMR CNRS 7338), Université de Technologie de Compiègne, Compiègne, France (https://bmbi.utc.fr)

Research group: Interactions Fluides Structures Biologiques (IFSB)

Supervisors:
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Scientific domains: Computer science, Mathematics, Physics, Biomedical engineering

Key words: Multiphysics simulations, Drug delivery, Capsules

Research Project: UC-DC : Ultrasonic-Controlled delivery from Drug Carriers (ANR-23-CE51-0057)

Research work: Capsules are closed membranes made of polymers protecting a fluid droplet. They are increasingly used in cosmetics and pharmaceutics to encapsulate active agents in order to accomplish controlled and targeted delivery. For example, in medicine, they are used to transport and release drugs or contrast agents to targeted sites within the human body. The delivery takes place either by mass transfer through the capsule membrane or by complete break-up of the entire capsule. Mass transfer from unbroken capsules have been extensively studied numerically at BMBI [1-7] as well as the evolution of damage and initiation of rupture on the membrane [8-10]. Experimental study of breakup has shown the fast release of the entire capsule cargo [11]. Triggering drug release from microcapsules ensures a controlled localized delivery of the active substances. Among all the possible triggering strategies, ultrasonic stimulation offers the advantages to be controllable at distance and not damaging for the surrounding cells.

The present project aims at modeling the sonication of microcapsules suspended in an external flow numerically, and accounting for the rupture of the capsule membrane when subjected to strong ultrasonic forces. The recruited person will participate in developing a new numerical method to model the rupture of the capsule membrane using physics-based approaches. The capsule will be modeled as a closed spring network, as done in Ref. [1], and the mechanism of brittle materials break-up will be implemented. The developed numerical method will be used to study capsule rupture as a function of the membrane elastic properties and the strengths of the applied ultrasonic stimulation and flow. Regular comparison of the theoretical and numerical results will be done to experimental results obtained by other partners of the ANR project to improve the models and help explain the observed phenomena.

Planned tasks and deliveries of the project:

Learning the fundamentals of the lattice Boltzmann method (LBM) and get familiar with the in-house computer code “lbm3d”, design and implementation of boundary conditions needed to compute flow induced by ultrasound, perform validation, convergence tests and benchmarking tests of the newly developed code that models ultrasonic forces,

Learning the fundamentals of the finite element method (FEM) needed to compute the mechanics of the capsule, and the immersed boundary method (IBM), needed to accomplish the fluid-structure interaction (FSI) with the Caps3D code [12], get familiar with both in house computer codes “Caps3D” and “ibmd3d”, coupling the structure with the ultrasound-flow solver, perform systematic numerical study of the dynamics and deformation of the capsule under ultrasonic forces, comparison with experimental results,

Study the capsule break-up event and the accompanied release of the capsule cargo, study the spatial distribution of the released molecules within blood vessel, and its absorption rate by the vessel wall and surrounding tissues.

Material resources: Powerful work station and access to High Performance Computing facilities

National collaborations: ENS Paris

Requirements: Good background in mathematics and physics, with skills in scientific coding and computing (C/C++, Fortran, Python, CUDA, MPI). MSc/PhD in Computer Science, Mechanical or Biomedical Engineering, with an interest in biomedical applications.

References:

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