Preface

As an emerging field of bio-science and bio-engineering, mechanobiology is a multidisciplinary research area that focuses on the interplay or interrelation between mechanical or thermodynamic forces and biological functions. This interplay is complex, and most of time, occurs across multiple time and length scales. Moreover, most biological systems are susceptible to slight alterations of thermodynamic conditions at room temperature, so that they can rapidly change from one state to another under slight thermal fluctuations. Using technical terminology, such systems are often referred to as a soft matter or soft matter systems.

The manifestation of biological soft matter in real life is complex, diverse and often highly sensitive to environmental conditions. By developing powerful computation or simulation approaches that can characterize and explore key mechanisms across the scales, we may gain a fundamental understanding of their bio-physical and bio-chemical responses. Eventually, such simulation tools, when used in concert with experimental techniques, will enable the prediction and perhaps manipulation of biological systems with key outcomes in life science, healthcare technology, and medicine. The objective of this special issue (CMES vol. 98, no. 1-3) is thus to compile and disseminate the state-of-the-art computation technologies that are used in mechanobiology or bio-medical engineering. Eventually, we hope that this will advance and promote the field of computational mechanobiolgy at the forefront of bioscience and life science.

The first contribution of the special issue is from Regueiro, Zhang, and Wozniak, who present a three-dimensional, large deformation, coupled finite element analysis of dynamic loading on soft biological tissues, which are modeled as biphasic (solid/fluid) porous media. This is an ambitious effort to bring the contemporary computational mechanics modeling and simulation techniques to solve biological problems. The next contribution is from Wang and Zhang, who combine a connectivity-free front tracking method and a moving contact line method to simulate blood spreading, and it can be used in bloodstain pattern analysis; this contribution is particularly important to forensic science and technology. In the third paper, Aggarwal, Chen, and Klug present a coarse-grain meshfree method to compute conformational change of proteins and their assemblies. This work is not only important as it addresses a challenging multi-scale problem, but also for its obvious applications in computational biology and biomaterials. In the fourth paper, Foucard, Pellegrino and Vernerey present their original work on a particle-based moving interface method for the study of the interactions between soft colloid particles and immersed fibrous networks. They particularly show how colloid deformability drastically affects their permeation through a porous network with potential applications in the filtration of complex biological fluids and the mechanobiology of cell-matrix interactions. Alford, Simkins, Rembert, and Hoyte then present their novel work on patient-specific modeling in urogynecology, in which they adopt a meshfree method to model and study mechanical deformation of the female pelvic floor that can be used as a diagnostic tool in clinic observation, this work reports the state-of-the-art technology in the patient-specific modeling. The sixth paper is contributed by Yalcinatas, Hu, Liu, and Voloshin, who use predictive simulation to shed light on the complex mechanics of cell spreading on a wavy surface. Based on a tensegrity model of the cell cytoskeleton, the authors numerically investigate the possible active mechanisms that control the spreading and alignment of the cell in terms of the surface waviness. The seventh paper of this special issue is authored by

Pradhan, Kalpana and Dinesh Katti, who present a multiscale modeling of collagen fibril in bone, in which they incorporate the material properties of collagen obtained from steered molecular dynamics into the finite element model of collagen fibril with the incorporation of crosslinks. Lin, Wang, and Zeng then proceed to the presentation of a geometrical model of cell division by using the Voronoi tessellation method. The idea is based on that fact that in most laboratory environment, the morphology of cell division resembles to geometrical configuration and structure of Voronoi cells. The ninth contribution of this issue then deals with the issue of the process of drug delivery in cells. In this context, Campello and Zohdi present a novel work on particle dynamics simulation of the bombardment of a stream of fine particles into a cell. The subsequent paper is a molecular dynamics study of ion diffusion through nanotubes that are embedded in cell membrane, which is authored by Tu, Lee, Zhang, and Li. Ion diffusion is a vital physiology process of cells, which is usually accomplished by various biological ion channels. This study is particular useful for artificial and synthetic ion channel and the cell probe device design. The next paper is a work by Zohdi, who presents a computational modeling framework for heat transfer processes in laser-induced dermal tissue removal, which is a procedure that has been extensively used in medical industry. Shim and Mithraratne then present a multiscale modeling approach for the study of mechano-activation patterns in nuclear factor-κB in skin. The impact of this work is timely as it brings a fundamental understanding on how the activation of NF-κB, an important precursor in developing melanoma, is dependent on mechanical stimulation of skin. The next contribution is from Hammond, Stewart, Younger, Solomon, and Bortz, and they study variable viscosity and density of biofilm by using an immersed boundary method, which is central to the mechanical response and fragmentation of a bacterial biofilm in shear flow. This paper is the first part of a systematic study of this very important practical problem in healthcare and bio-engineering. Finally, the last contribution is from Budyn, Bilagi, Subramanian, Orias, and Inoue -- a team of computational specialists, experimentalists and medical professionals who present a multiscale protocol to prepare surfaces of human endplate specimens for morphometric characterization at the tissue and cell levels. Their approach is based on a hybrid multiscale simulation/experimentation method that may have significant practical implications.

Most of the authors appearing in this volume are younger researchers who are actively working on problems related to computational mechnobiology or bio-mechanics. Importantly, the issue also features a number of contributors who are healthcare professionals, and they have established collaborations with computational specialists in order to solve practical problems in medical diagnosis and treatment. Most of the contributions presented here are novel and by bringing them together into one volume, we wish to advance the computational technology and its applications to biological problems. We hope that this issue will be successful at showing how the field of computational science and engineering is critical to solving challenging biological problems and how it will aid the development of new solutions in healthcare and medicine.

Franck Vernerey and Shaofan Li

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